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MATHEMATICAL MODEL OF THE ELECTRODIALYSIS PROCESS

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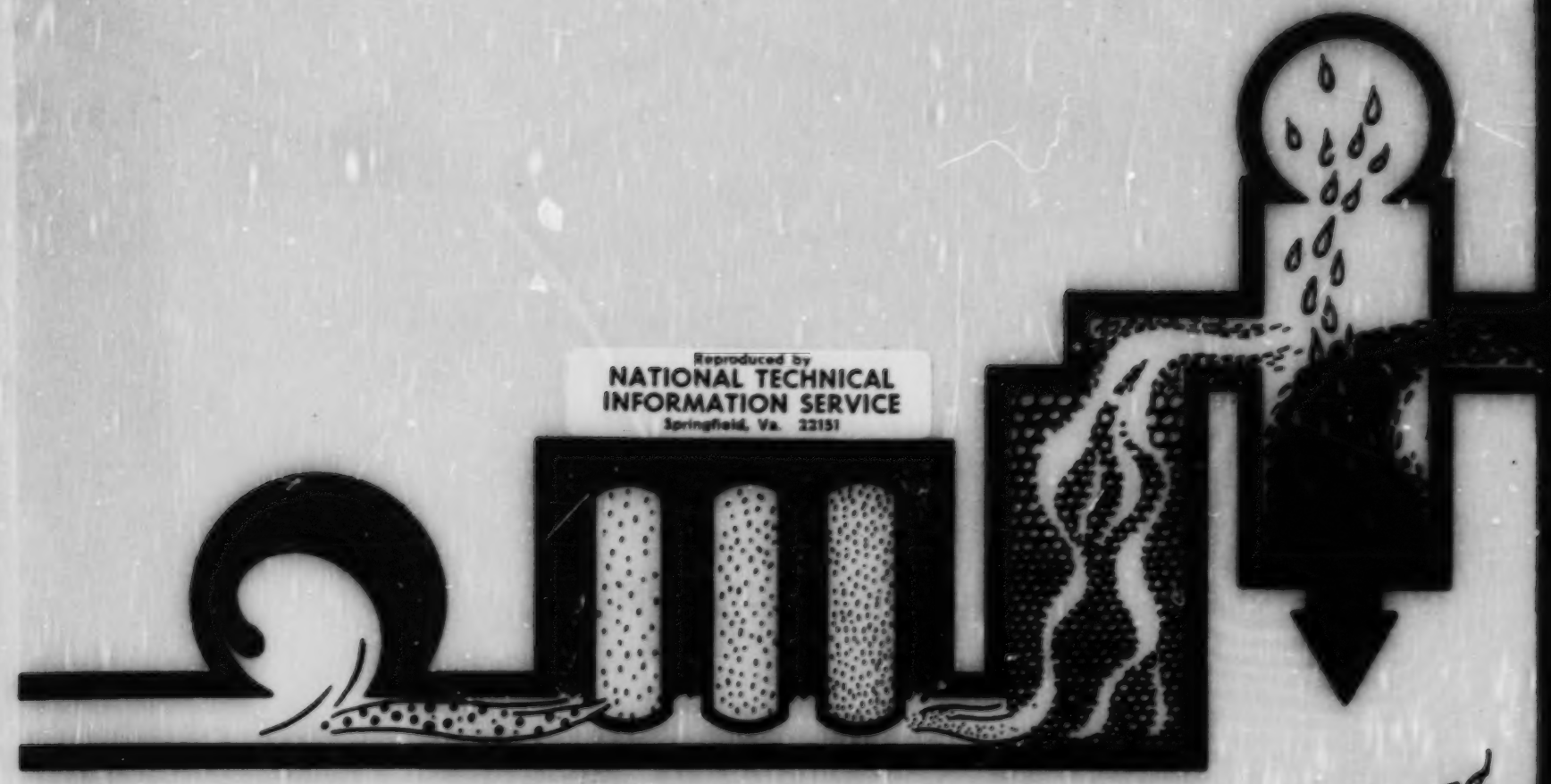

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MATHEMATICAL MODEL OF THE ELECTRODIALYSIS PROCESS

by

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for the

FEDERAL WATER QUALITY ADMINISTRATION

DEPARTMENT OF THE INTERIOR

Program #17090 FTA
Contract #14-12-410
FWQA Project Officer, J. F. Roesler
Advanced Waste Treatment Research Laboratory
Cincinnati, Ohio
July, 1969

For sale by the Superintendent of Documents, U.S. Government Printing Office
Washington, D.C. 20402 - Price 70 cents

1 Accession Number	2 Subject Field & Group	SELECTED WATER RESOURCES ABSTRACTS INPUT TRANSACTION FORM
W71-09525	05D	

5 Organization
Process Research, Incorporated, Cambridge, Massachusetts

6 Title
MATHEMATICAL MODEL OF THE ELECTRODIALYSIS PROCESS,

10 Author(s)	16 Project Designation	21 Note
Pruyn, Kenneth T. Harrington, Joseph J. Smith, J. Douglas	FWQA Contract #14-12-410, Program #17090 FTA 07/69	I67.13/4: 17090 FTA 07/69 Copy available from GPO Sup Doc as , $.70 ; ~~also available from~~ NTIS as PB , ~~$3.00~~

22 Citation
Water Pollution Control Research Series ~~ORD-17090FTA07/69~~, July 1969, 70 p, ~~illus.~~
3 fig, 3 tab, 18 ref

23 Descriptors (Starred First)
*Computer simulation, *Mathematical models, Feasibility studies, Cost analysis, Electrodialysis, Separation techniques, Membrane processes, Semipermeable membranes, Anions, Cations, Demineralization, Desalination, Resistivity, Flow, Acid, Storage, Instrumentation, Pipes, Pumps, Waste water treatment

25 Identifiers (Starred First)
~~None~~ desalination

27 Abstract An electrodialysis unit was established as a control volume, and material balances around the control volume were formulated, involving input and output flows, types of charged particles to be exchanged, concentrations of charged particles, and percentage removal of individual ions as well as percentage removals of total ions. Significant parameters involved included spacer design geometry, membrane properties (resistivity, current efficiency, separation factors, etc.) and mode of operation of the stack (current density, products stream concentration, waste/product ratio, waste stream pH, etc.). Performance equations were then formulated for resistivity, D.C. power input, current efficiency, number of stacks required, and the pumping headloss. Cost analyses were then derived to include: (1) electrodialysis stacks, stack piping, distribution piping, and pumps for stack related costs; (2) rectifiers and process electrical for D.C. power costs; and (3) acid storage tanks, acid feed pumps, instruments, and miscellaneous equipment for auxiliary costs. Equations derived for capital costs, were based on the January 1965 Engineering News-Record cost index. Operational costs were estimated and evaluated in the same manner. The program was run for plants of 1, 10, and 100 MGD, with capital and operating costs being $164,620 and 7.07¢/1000 gallons respectively for a 1 MGD plant. Program flow charts as well as actual computer outputs are presented. (Lowry-Texas)

(WRSIC abstract)

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WR 102 (REV. JULY 1969)
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Electrodialysis Process Description

The electrodialysis process removes ionized salts and minerals from water by the migration of ions through plastic ion-transfer membranes, under the influence of a D. C. electrical field. Commercially available electrodialysis membranes are thin sheets (4-40 mils thick) of cross-linked organic polymeric materials. These membranes are similar in composition to granular ion exchange resins, except for their physical form. They commonly contain 40-50%, by weight, of water which is distributed in extremely fine pores honeycombing the plastic structure. The size of these pores has been estimated at 10-100 A°. For the salt concentrations common to advanced waste treatment applications, water transfer through these membranes will be virtually zero. Two types of membranes are necessary to the process:

1) Cation permeable membranes, which will permit the passage of cations but, because of the Donnan exclusion principle, will prevent the passage of anions; and
2) Anion permeable membranes, which for the same reason will allow the passage of anions but not cations.

If two metal electrodes are placed in an aqueous salt solution and electrical current is passed between them, all of the negative ions will move toward the positive electrode and all of the positive ions will move toward the negative electrode. If, now, alternative cation and anion permeable membranes are interposed between the electrodes, the movement of the ions in the electrical field will be seriously restricted. Half of the ions will be able to move through one type of membrane barrier and half will not; no ion will be able to move through more than one barrier. This is illustrated in Figure 1. In this figure, cations from compartments whose left boundary is a cation membrane (compartments 2, 4, 6, 8, 10, etc.) will move one compartment to the left but must then stop because the second membrane to be encountered will be an anion membrane, which is impermeable to cations. Conversely, anions from compartments whose right boundary is an anion membrane (compartments 2, 4, 6, 8, 10, etc.) will move one compartment to the right, but must then stop because the second membrane they encounter will be a cation membrane and impermeable to anions. The net result, therefore, of the interposition of the alternating cation and anion permeable membranes between the electrodes is the creation of two types of compartments:

diluting compartments (i.e., 2, 4, 6, 8, 10) which will lose ions; and concentrating compartments (i.e., 3, 5, 7, 9) which will gain ions.

The extent of salt removal, or demineralization, obtained in the diluting compartments will depend upon the amount of electrical current passed, the concentration of ions present in the feed solution, and the flow rate of the feed solution through the equipment. All ions are not, however, removed at identical rates, some moving preferentially faster than others. This preferential, or selective, removal of certain ions is described here by a Separation Factor. The Separation Factor for each ion is the ratio of its percentage reduction to the total concentration reduction through the process.

In compartments 1 and 11, electrode reactions take place. Hydrogen gas and hydroxide ions (OH^-) are produced at the cathode, or negative, electrode; oxygen or chlorine gas and hydrogen ions (H^+) are produced at the anode, or positive electrode. The effluent from these electrode compartments may, in some situations, be useful for chemical operations, being sources, respectively, of base and acid. The gases produced at the electrodes may be used for disinfection, or as a source of fuel. For purposes of this model, the cathode and anode waste streams will be mixed with the concentrated brine and be considered a part of the total waste stream.

The mathematical model developed here for the electrodialysis process represents an attempt to describe the present, moderately well documented state of the art of commercially available equipment and operating practice. Current state of the art has been established from site visits and discussions with operating personnel at various electrodialysis installations in this country, i.e., Lebanon, Ohio; Pomona, California; Port Mansfield, Texas; etc.; from the literature and from our own experience.

The modeling of presently available equipment in no way implies that such equipment is optimally designed or operated for waste water treatment applications. Our own independent studies, in fact, indicate rather the opposite. Our design optimization programs, for instance, suggest that modifications of flow path geometry, i.e., thickness and/or width, could result in greatly reduced membrane area and D.C. power requirements. Our membrane fouling studies have indicated modes of operation, or pretreatments, which would further reduce membrane area and maintenance requirements.

The potential cost reductions, on the order of one-half of present cost estimates, to be gained through these various design and operating modifications are sufficient to justify

their further examination and documentation on something larger than a laboratory scale.

Such modifications have not been included in the model developed here, because inadequate field experience has been obtained to warrant their inclusion as present "state of the art". An attempt, however, has been made to express this model in sufficiently general terms as to readily facilitate their later inclusion.

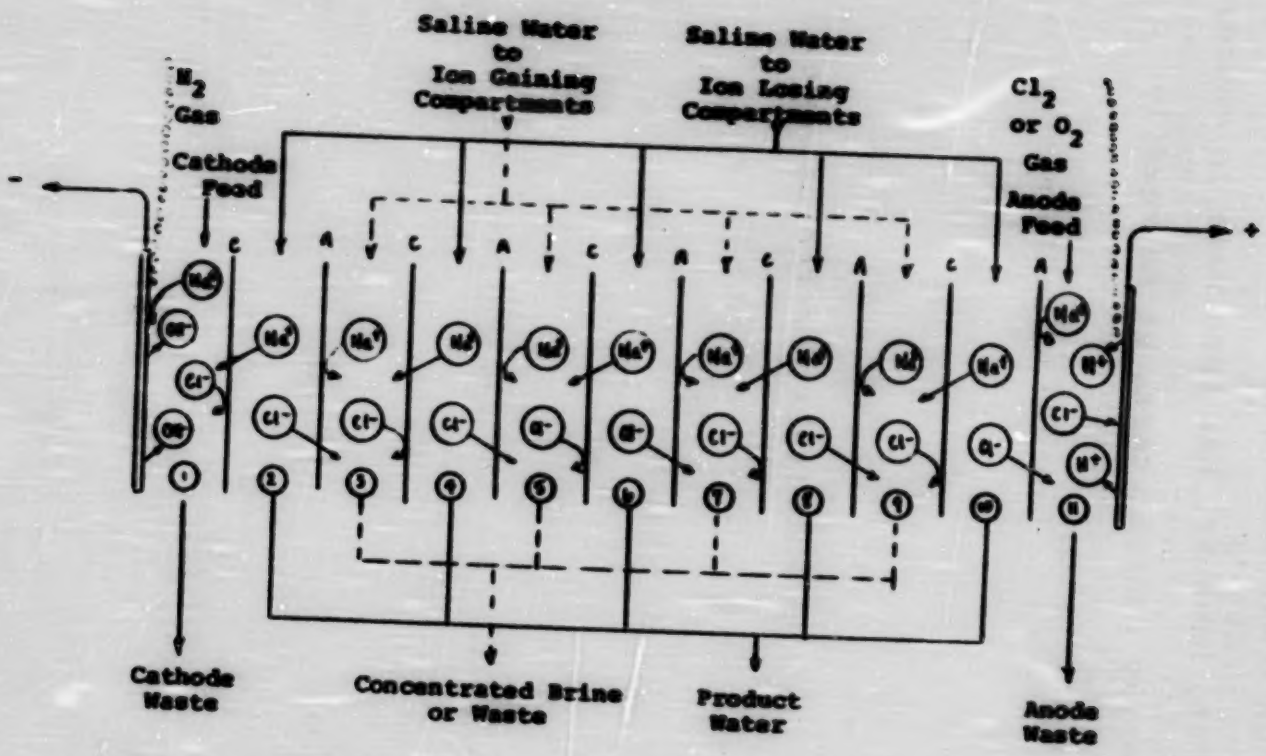

Saline Water to Ion Gaining Compartments
Saline Water to Ion Losing Compartments
H_2 Gas Cathode Feed
Cl_2 or O_2 Gas Anode Feed
Cathode Waste
Concentrated Brine or Waste
Product Water
Anode Waste
Compartment Number (see text)
Any Cation (Positive Ion) Like Sodium
Any Anion (Negative Ion) Like Chloride
C Cation Membrane
A Anion Membrane

FIGURE 1

BASIC ION AND WATER FLOW IN ELECTRODIALYSIS STACK

Electrodialysis Equipment

The physical structure in which these demineralization operations are carried out is called a membrane "stack". Such a membrane stack is illustrated, in an expanded view, in Figure 2. The stack consists of alternative anion and cation permeable membranes, spacers, electrodes, end blocks for making inlet and outlet manifold connections, heavy steel end plates, and tie rods to provide uniform sealing pressure.

The electrodes are thin metal sheets, stainless steel or Hastelloy C being typical materials for the cathode. Graphite, or platinum coated sheets of tantalum or titanium, are typical materials for the anode.

The spacers are probably the most important component in the electrodialysis stack, after the membranes themselves. They:

1) serve as gaskets, containing the water between the membranes;
2) separate the thin, flexible membranes a constant distance from each other; and
3) direct the flow of water across the surface of the membranes.

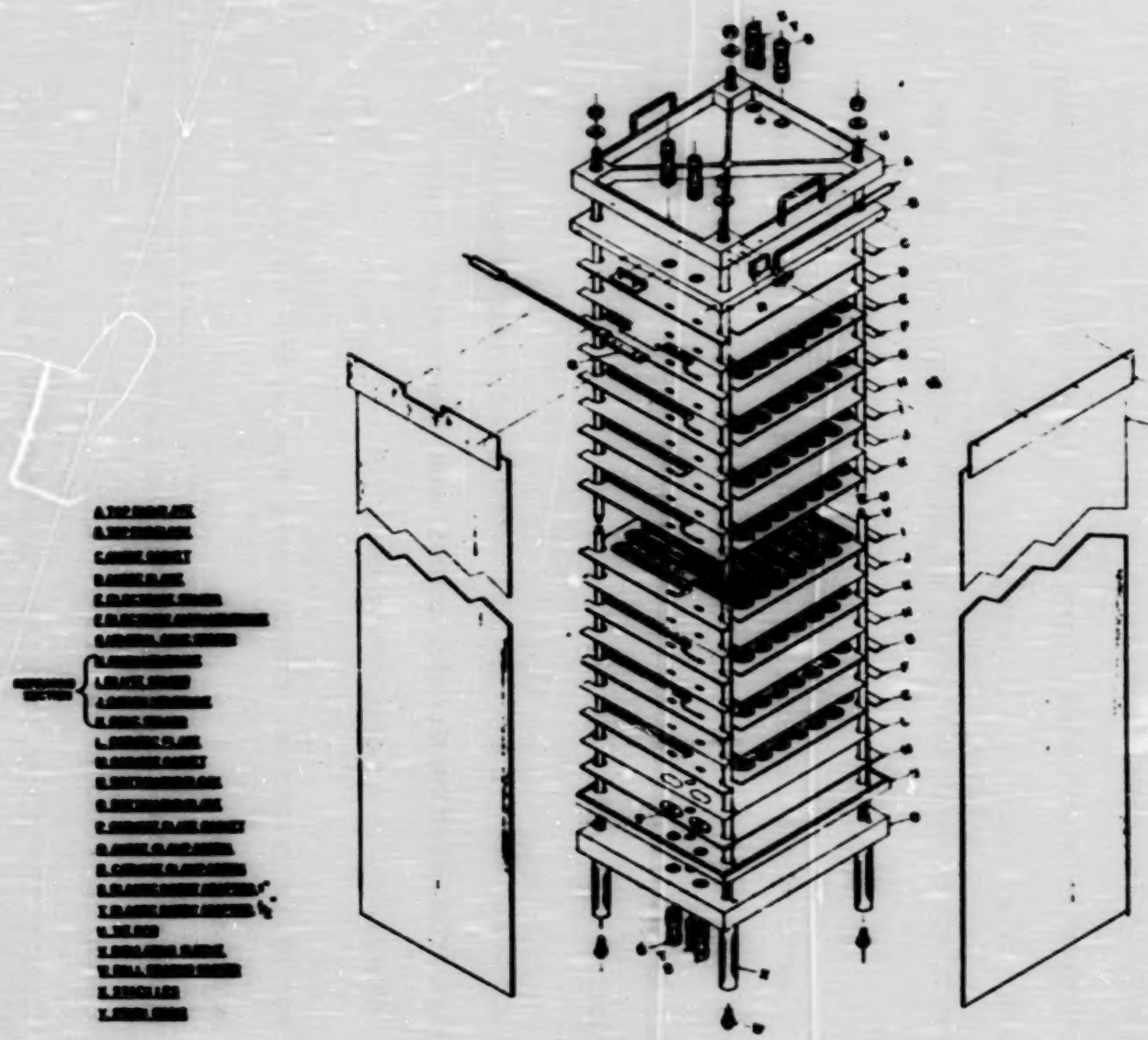


Figure 2

Expanded View of Electrodialysis Stack

A good spacer will be designed to provide an even distribution of flow, and to promote sufficient turbulence at the membrane-liquid interface to avoid the formation of polarization films (to be discussed later). It has been suggested that by far the greatest immediate process improvement, or cost reduction, is to be found through optimal design of the geometry of these spacers (see OSW R&D Report No. 325).

There are two general types of spacer designs used in present commercially available equipment: the so-called "sheet flow" design, as used in the Asahi Chemical electrodialysis plant at Webster, S. D.; and the so-called "tortuous-path" design, as used in the Ionics, Inc., plant at Buckeye, Arizona. The spacers shown in Figure 2 are of the tortuous-path variety, the illustration being that of an early Ionics, Inc. stack design.

Spacers are fabricated from sheets of electrical insulating, plastic materials having good gasketing properties. Common materials are plasticized polyvinyl chloride, polyethylene or rubber-styrene compounds. In the tortuous-path type spacer illustrated here, a flow path for the salt solution is die-cut into one sheet of spacer material, along with manifold holes and appropriate connections between manifold holes and flow path. In the sheet-flow type spacer, a

perimeter gasket containing the manifold holes and connections to the flow path are die cut from sheets of gasket material. Into the center of these perimeter gaskets, then, are inserted plastic "screens", or mats, which provide the necessary membrane support while still permitting hydraulic flow through the compartments. Common insert support materials have been expanded, or corrugated and perforated, PVC or polypropylene.

Present commercially available electrodialysis stacks contain approximately 500 membranes, or 250 anion-cation membrane pairs. These stacks have hydraulic capacities of the order of 250,000 gpd and conventionally provide a salt reduction, or demineralization, or 40-60%. The concentrate, or brine, stream is generally recirculated through the stack at the same flow rate as the feed stream so as to minimize pressure differentials across the somewhat fragile membranes.

Mathematical Model

An electrodialysis process flow schematic, upon which the mathematical model is based, is shown in Figure 3. The development of the model follows the outline suggested in Publication No. WP-20-9, "Preliminary Design and Simulation of Conventional Waste Water Renovation Systems Using the Digital Computer".

By writing material balances around the control volume "A" in Figure 3, the following equations can be derived for flow and salt concentrations:

$$Q_1 + Q_9 = Q_3 + Q_7 \tag{1}$$

and:

$$Q_1C_1 + Q_9C_9 = Q_3C_3 + Q_7C_7 \tag{2}$$

Assuming no water transport across the membranes, material balances written around control volumes "B" and "C" will establish the following relationships:

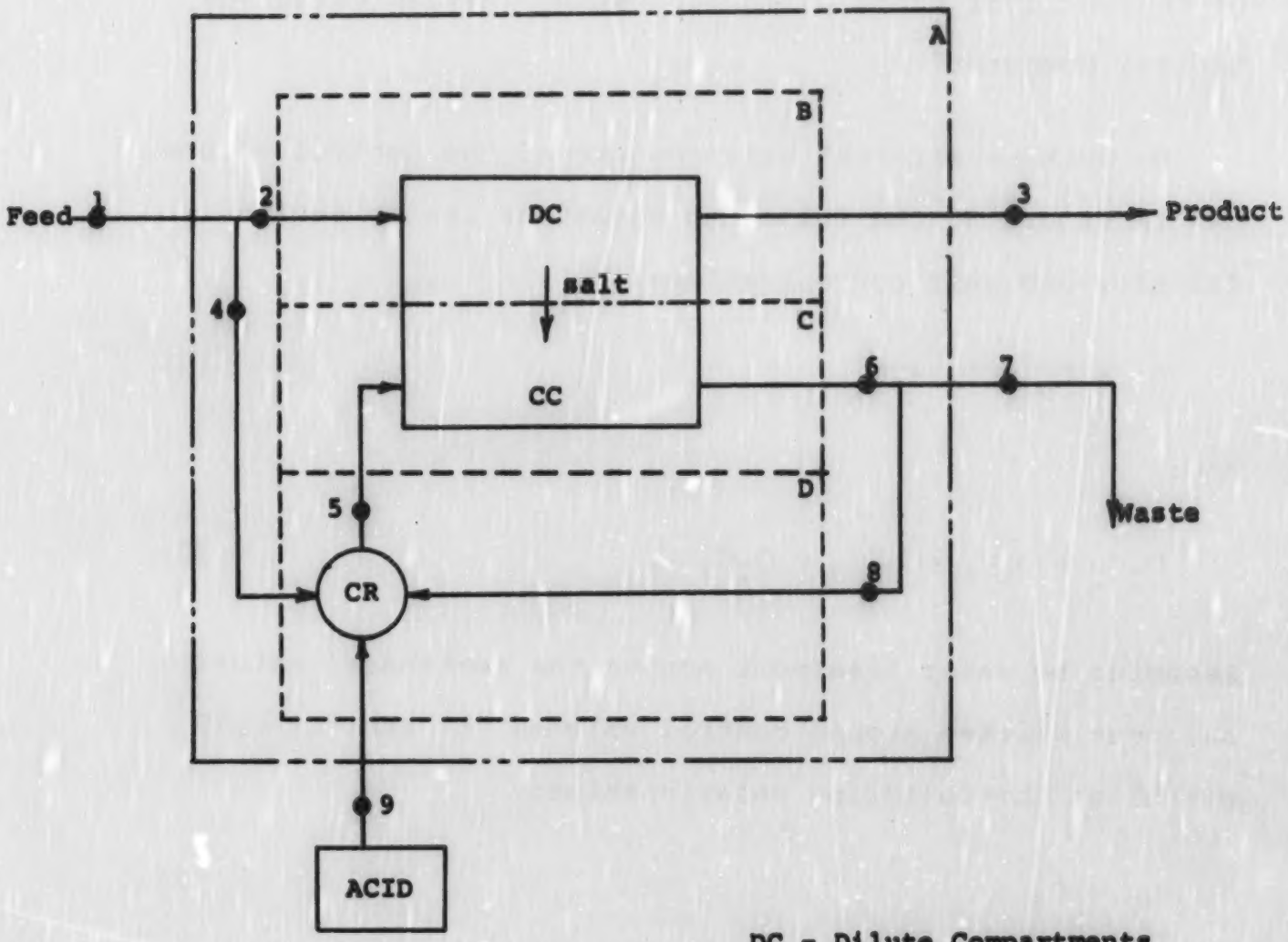
$$Q_2 = Q_3 \tag{3}$$

and:

$$Q_5 = Q_6. \tag{4}$$

FIGURE 3

Electrodialysis Process Flow Sheet



DC - Dilute Compartments
CC - Concentrate Compartments
CR - Concentrate Recycle
ACID - Acid Feed

If FRACT equals the fraction of total influent salt transferred from diluting to concentrating compartments:

$$C_3 = C_2 \ (1\text{-FRACT}) \tag{5}$$

$$C_6 = C_5 + \frac{Q_2}{Q_5} C_2 \text{FRACT} \tag{6}$$

The fraction transferred of any ionic species is the product of the total fractional salt transferred (FRACT) and that ion's separation factor α_i, where α_i is the ratio of the percentage removal of ion species i to the percentage removal of total salt:

$$C_{3i} = C_{2i}(1-\alpha_i \text{FRACT}) \tag{5a}$$

$$C_{6i} = C_{5i} + \frac{Q_2}{Q_5} C_{2i} \alpha_i \text{FRACT} \tag{6a}$$

If, as is customary, the stack is operated with equal flow rates through both the diluting and concentrating compartments:

$$Q_5 = Q_2 \tag{7}$$

and:

$$C_6 = C_5 + C_2 \text{FRACT} \tag{8}$$

Writing material balances around control volume "D":

$$Q_5 = Q_4 + Q_8 + Q_9 \tag{9}$$

and:

$$C_5 Q_5 = C_4 Q_4 + C_8 Q_8 + C_9 Q_9 \tag{10}$$

Also:

$$C_1 = C_2 = C_4 \tag{11}$$

and:

$$C_6 = C_7 = C_8 \tag{12}$$

The above equations, then, can be combined to yield:

$$C_7 = C_1\left(\frac{Q_4}{Q_7} + \frac{Q_2 FRACT}{Q_7}\right) + C_9 \frac{Q_9}{Q_7} \tag{13}$$

In this model, the <u>stream vectors</u> include stream identification numbers, volume flow rates (MGD), and concentrations of the various contaminants pertinent to the electrodialysis process. In the latter regard, the classification scheme for contaminants is somewhat different from those generally pertinent to other waste stream processes, in that primary emphasis is placed on the composition of inorganic, rather than organic, materials. The concentrations of each ionic species present are specified in the stream vectors. The electrodialysis stream vector is:

<u>Contents of Stream Vector for Electrodialysis</u>

Row No.	Descriptive Parameter	Fortran Variable Names
2	Volume Flow, MGD	SMATX(2,I),Q
18	Concentration of Dissolved Sodium	SMATX(18,I),PNA
19	Concentration of Dissolved Potassium	SMATX(19,I),PK
20	Concentration of Dissolved Calcium	SMATX(20,I),PCA
21	Concentration of Dissolved Magnesium	SMATX(21,I),PMG
22	Concentration of Dissolved Ammonium	SMATX(22,I),PNH4
23	Concentration of Dissolved Chloride	SMATX(23,I),PCL
24	Concentration of Dissolved Bicarbonate	SMATX(24,I),PHCO3
25	Concentration of Dissolved Sulfate	SMATX(25,I),PSO4
26	Concentration of Dissolved Nitrate	SMATX(26,I),PNO3
27	Concentration of Dissolved Phosphate	SMATX(27,I),PPO4

The decision vector for the electrodialysis process contains parameters describing:

1) spacer design geometry, i.e., flow path thickness;
2) membrane properties, i.e., resistivity, current efficiency and separation factors (see WP-20-AWTR-18) for each of the ions present in the feed stream; and
3) mode of operation of the stack, i.e., current density, product stream concentration, waste/product ratio, waste stream pH, etc.

The electrodialysis decision vector is:

Contents of Decision Vector for Electrodialysis

Row No.	Descriptive Parameter	Fortran Variable Names
1	Total Dissolved Inorganic Solids, Product Stream, ppm	DMATX(1,N),PPMOU
2	Membrane Spacer Thickness, cm	DMATX(2,N),TKNS
3	Ratio of Spacer Thickness to Mesh Spacing	DMATX(3,N),TDEL
4	Input Stream Temperature, Deg-F	DMATX(4,N),T
5	Cation Membrane Resistivity, ohm-sq.cm	DMATX(5,N),RCM
6	Anion Membrane Resistivity, ohm-sq.cm	DMATX(6,N),RAM
7	Current Efficiency	DMATX(7,N),E
8	Limiting Current Density Parameter	DMATX(8,N),CURK
9	Desired Waste/Product Stream Volume Ratio	DMATX(9,N),GAMMA
10	Maximum Allowable Waste/Product Stream Volume Ratio	DMATX(10,N),GMAX
11	Max Allowable Hydrogen Ion Concentration in Waste Stream	DMATX(11,N),HMAX
12	Cosine of Mesh Angle, Theta	DMATX(12,N),COTHE
13	Separation Factor, Sodium	DMATX(13,N),ANA
14	Separation Factor, Potassium	DMATX(14,N),AK
15	Separation Factor, Calcium	DMATX(15,N),ACA
16	Excess Capacity Factor	DMATX(16,N),ECF
17	Separation Factor, Magnesium	DMATX(17,N),AMG
18	Separation Factor, Ammonium	DMATX(18,N),ANH4
19	Separation Factor, Chloride	DMATX(19,N),ACL
20	Separation Factor, Bicarbonate	DMATX(20,N),AHCO3
21	Separation Factor, Sulfate	DMATX(21,N),ASO4
22	Separation Factor, Nitrate	DMATX(22,N),ANO3
23	Separation Factor, Phosphate	DMATX(23,N),APO4

Electrodialysis Performance Equations

The influent salt concentration at Station 1, and the required effluent salt concentration at Station 3, are supplied to the program as input. The waste stream salt concentration at Station 7 is calculated as the maximum concentration that can be achieved without precipitating calcium (as carbonate or sulfate), or as the concentration resulting from the lowest desirable O_7 to O_3 ratio supplied as input, whichever is the smaller.

The repetitive physical unit of an electrodialysis stack is called a cell-pair and consists of a diluting compartment, concentrating compartment, and two membranes. The average areal resistivity (ohm-cm^2) of the cell pair, as derived in Appendix A, is:

$$RPA = RM + \frac{TKNS}{FRACT*CLAM*C_1} \ln\left(\frac{C_7/C_1}{(1-FRACT)(C_7/C_1-FRACT)}\right) \quad (14)$$

The areal resistivity (ohm-cm^2) at the effluent end of the cell-pair is:

$$RPO = RM + \frac{TKNS}{CLAM}\left(\frac{1}{C_3} + \frac{1}{C_7}\right) \quad (15)$$

The total electrical resistance of one cell-pair (ohm) is the average areal resistivity divided by the effective transfer area per membrane:

$$RP = \frac{RPA}{AM} \tag{16}$$

The D.C. current (amperes) required to remove a given amount of salt is obtained from Faraday's Law:

$$I = \frac{96{,}500*(C_1-C_3)*Q_3*43.9}{E*NCP} \tag{17}$$

where E is the current efficiency of the process and NCP is the number of cell-pairs per stack.

The D.C. power (kw) requirement then is obtained from Ohm's Law:

$$EDPWR = \frac{I*NCP*EP}{1000}, \tag{18}$$

where EP is the applied cell-pair voltage.

The number of electrodialysis stacks required is also obtained from Ohm's Law:

$$NSTK = \frac{I*RP}{EP} \tag{19}$$

There, in general, is a limiting value assigned to EP, that is a complex function of the hydrodynamic design and

operation of the particular electrodialysis equipment being used. The expression for the polarization parameter, XICD, is derived in Appendix A; the appropriate design value for EP is obtained from Ohm's Law:

$$EP = \frac{XICD*C_3*RPO}{1000} \qquad (20)$$

The pumping head loss (ft H_2O) through the electrodialysis stacks is calculated:

$$STKHD = 30 + PGRAD*LENGTH \qquad (21)$$

where 30 ft is the contribution due to piping and manifold losses, PGRAD is derived in Appendix A, and LENGTH is the flow path length defined as the ratio of membrane area to flow path width.

Electrodialysis Process Cost Functions

The goal of this effort was to develop simple relationships that give a good approximation to the cost of commercially available equipment. Data on cost of actual operating electrodialysis plants were taken from OSW R&D Progress Report No. 134, "An Engineering Evaluation of the Electrodialysis Process Adapted for Computer Methods for Water Desalination Plants", Mason-Rust, Webster, South Dakota (1965). Relationships among the various cost items, particularly relative magnitudes, which were useful in making functional approximations were given by OSW R&D Progress Report No. 325, "Hydraulic Design Optimization of the Electrodialysis Process", by Process Research, Incorporated (1967). Some values used were in accordance with conventions recommended by the Office of Saline Water and are so noted where used in this development. Capital costs are assumed to be referred to the Engineering News - Record Cost Index January 1965.

Capital Costs*

It was generally convenient to divide electrodialysis capital cost items into three related groups and develop separate cost equations for each group. The groups are stack related equipment, D.C. power related equipment, and auxiliary equipment.

Stack related costs include:

Electrodialysis Stacks

Stack Piping

Distribution Piping

Pumps, Dilute Stream and Concentrate Recycle.

Pumps for delivering feed water from the source to the plant, and pumps for carrying off product water and waste water which are usually included in electrodialysis plant cost calculations were not included here.

D.C. power costs include:

Rectifiers

Process Electrical.

Auxiliary costs include:

Acid Storage Tank

Acid Feed Pumps

Instruments

Miscellaneous Equipment.

*Publisher's Note: Estimates of capital and operating and maintenance cost presented in this report are low compared to other authoritative sources. For the most reliable cost information equipment manufacturers should be consulted.

The cost of a building to house the plant would be included in the cost of an electrodialysis plant operating on its own. As a part of a waste water treatment facility the building space would be shared. The building area required by the ED process itself is calculated and passed along to the executive program so that it may be combined with all other building area requirements. Engineering cost, contractor's profit, contingencies and omissions, and cost of land are not included because they are handled by the executive system.

Electrodialysis stack materials costs were based on the following:

Membrane Cost	$1.00-3.00/sq. ft.
Membrane Size	5-10 sq/ ft.
Membrane Pairs/Stack	250-300
Spacers	$.60-1.00 sq. ft.
Anode	$26.00/sq. ft.
Cathode	$4.43/sq. ft.
End Plate/End Block	$114.60/sq. ft.
Stack Hardware	$72.20/sq. ft.
Manufacturers Assembly Cost	$4.00/sq. ft. Membrane Area
Stack Erection Labor	160 man-hrs.
Erection Labor Cost	$4.50/hr.
Payroll Extras	15%
General & Administrative	30%

The last two values, payroll extras and general administrative overhead follow OSW conventions.

Combining typical values from the foregoing table gives an erected stack cost as:

(2 x 275 x (1.00 + 3.00 + 4.00) + 26.00 + 4.43 + 2 x 114.60 + 72.20) x 5.0 + 160 x 4.50 x 1.15 x 1.30 = $24,700/stack

Stack piping = $750/stack

Distribution piping = $200/stack.

Cost of pumps depends on the capacity of the pumps. Flow in both the dilute and concentrate stream are essentially equal and are given by:

$$Q_3 = Q_6 = Q_1 - Q_7 \qquad (22)$$

The following values enter into pump costs:

Minimum number of concentrate pumps	2
Minimum number of dilute stream pumps	2
Base cost, stainless steel pump	$1800
Base cost, cast iron pump	$1400
Power cost, stainless steel pump	$52.50/HP
Power cost, cast iron pump	$30.30/HP
Stack piping head loss	30 ft.
Pump size scale factor	9.1

Cost of pumps is given by:

$$(2 \times 1400 + 30.30 \times STKHD \times Q_3/5.7) \times (2 \times 9.1/Q_3)^{0.2} + (2 \times 1800 + 52.50 \times STKHD \times Q_3/5.7) \times (2 \times 9.1/Q_3)^{0.2} = [6400 + 14.5 \times Q_3 \times STKHD] \times (18.2/Q_3)^{0.2}$$

where the exponent 0.2 is a scale factor for pump costs, and STKHD is the head loss through the stack and its associated piping.

A factor of 1.4 is applied to each item other than stacks to account for erection labor. A factor of 1.05 is applied to account for miscellaneous equipment. Combining all of the foregoing costs gives

$$CSTK = 1.05 \times 24700 \times XNSTK + 1.05 \times 1.4 \times (750 + 200) XNSTK + 1.05 \times 1.4 \times [6400 + 14.5 \times Q_3 \times STKHD] \times (18.2/Q_3)^{0.2} \quad (23)$$

where XNSTK = the number of stacks in the required plant, and
CSTK = the total capital cost of stack related items.

Equation (23) reduces to

$$CSTK = 27330 \times XNSTK + [16800 + 38.08 \times Q_3 \times STKHD] \times Q_3^{-0.2} \quad (24)$$

D.C. power related items include rectifiers and other process electrical equipment. Rectifier cost is made up of

Rectifier Base	$2700
Rectifier Power Cost	$63/KW
Number of Stacks/Rectifier	4

So that rectifier cost is:

$$(2700/4) \times XNSTK + 63 \times EDPWR$$

where EDPWR is electrodialysis power in kilowatts.

Process electrical cost is given as

$600/stack + $40/KW of D.C. power

Combining D.C. power items gives

$$CDC = 1.05 \times 1.4 \times [(2700/4 + 600) \times XNSTK + (63 + 40) \times EDPWR] \quad (25)$$

which reduces to

$$CDC = 1874.25 \times XNSTK + 151.41 \times EDPWR \quad (26)$$

Auxiliary equipment includes acid feed pumps, storage for acid and process instrumentation. Data given by Mason-Rust for the cost of acid storage tanks as a function of tank capacity lead to the following relationship:

$$\text{Tank Cost} = .0013 \times (\text{TANK SIZE})^{.715}$$

The size required to hold a 14 day supply is

$$14 \times Q_9 \times 10^6$$

Combining these two gives:

$$.0013 \times (14 \times Q_9 \times 10^6)^{.715}$$

or

$$167.3 \times Q_9^{.715}$$

Acid feed pump costs are based on the following values:

Number of Pumps	2
Pump Base Cost	$640
Pump Capacity	$101.90/GAL/DAY

so that cost is given by

$$2 \times 640 + 101.9 \times 10^6 \times Q_9$$

Mason-Rust suggests the following function for process instrumentation:

$$9600 + 750 \times \text{XNSTK} \times (\text{XNSTK}/4)^{-.17}$$

where \$9600 is the base cost and \$750 is the cost per stack for a small plant with 4 stacks and

$$(XNSTK/4)^{-.17}$$

is a scale factor to adjust down the unit cost of stack instrumentation in very large plants.

Total auxiliary equipment cost, CAUX, is given by combining the previous three costs

$$CAUX = 1.05 \times 1.4 \times [167.3 \times Q_9^{.715} + 1280 + 101.9 \times 10^6 \times Q_9 + 9600 + 750 \times XNSTK \times (XNSTK/4)^{-.17} \quad (27)$$

which reduces to

$$CAUX = 15993.6 + 149.79 \times 10^6 \times Q_9 + 245.9 \times Q_9^{.715} + 1102.5 \times XNSTK \times (XNSTK/4)^{-.17} \quad (28)$$

The total electrodialysis plant capital cost, then, is the sum of the stack, D.C. power and auxiliary equipment related costs,

$$CCAP = CSTK + CDC + CAUX \quad (29)$$

Operating Costs

Operating costs for the electrodialysis process consist of electrical power, membrane replacement, and other costs.

Pumping power is

$$STKHD \times (Q_3 + Q_6 \times CKWH \times 3.15 \times 365/.827$$

$$2780.5 \times STKHD \times Q_3 \times CKWH$$

where

$$Q_3 = Q_6$$

and electrodialysis power is

$$EDPWR \times CKWH \times 24 \times 365/.9$$

so that total power cost, CPWR, is:

$$CPWR = (2780.5 \times STKHD \times Q_3 + 9733.33 \times EDPWR) \times CKWH \quad (30)$$

Membrane replacement and stack tear-down costs are based on a membrane life of five years and stack disassembly frequency of six times per year. In waste water treatment applications operating conditions could be such that these figures would be very much different than would actually be experienced.

Based on a labor rate of $3.50/hr. and a stack disassembly time of 8 hrs./stack teardown cost is:

$$3.50 \times 8 \times 6 \times 1.15 \times 1.30 \times XNSTK$$

and membrane cost is

$$6.00 \times 5 \times 275 \times .2 \times XNSTK$$

so that membrane replace cost, CREP, is

$$CREP = 1900 \times XNSTK \qquad (31)$$

Other costs include:

Chemicals (Sulfuric Acid)

Operating Labor

Maintenance Materials

Using an acid cost of $30/ton, the cost of acid is:

$$30 \times 7619.7 \times Q_9 \times 365 = \underline{83.44 \times 10^6} \times Q_9$$

Operating labor is

$$1.15 \times 1.30 \times 3.50 \times (5.9 \times Q_3^{.725}) \times 365 = \underline{11268} \times Q_3^{.725}$$

where the exponent 0.725 is a scaling factor for large sized plants.

Conforming approximately to OSW suggested costing procedures, maintenance materials and supplies are estimated as 0.35% of plant cost, or in this case

$$.0035 \times (CSTK + CDC + CAUX)$$

Combining the preceding expressions gives total other costs, COT, as:

$$COT = 83.44 \times 10^6 \times Q_9 + 11268 \times Q_3^{.725} + .0035 \times [CSTK + CDC + CAUX] \quad (32)$$

Electrodialysis plant operating costs are the sum of electrical power, membrane replacement, and other related costs,

$$CTOP = CPWR + CREP + COT \quad (33)$$

Building area, ABLDG, required to include stacks, pumps and piping, instruments, membrane and parts storage and chemicals is based upon the following:

Chemicals

$$37 + (Q_3 \times 10^6)^{.33}$$

Membrane and parts storage

$$55 + (Q_3 \times 10^6)^{.4}$$

Instruments

$$(Q_3 \times 10^6)^{.33}$$

Pumps and Piping

$$60 + 20.36 \times Q_3$$

and Stacks

$$127.5 \times XNSTK$$

Combining the above gives

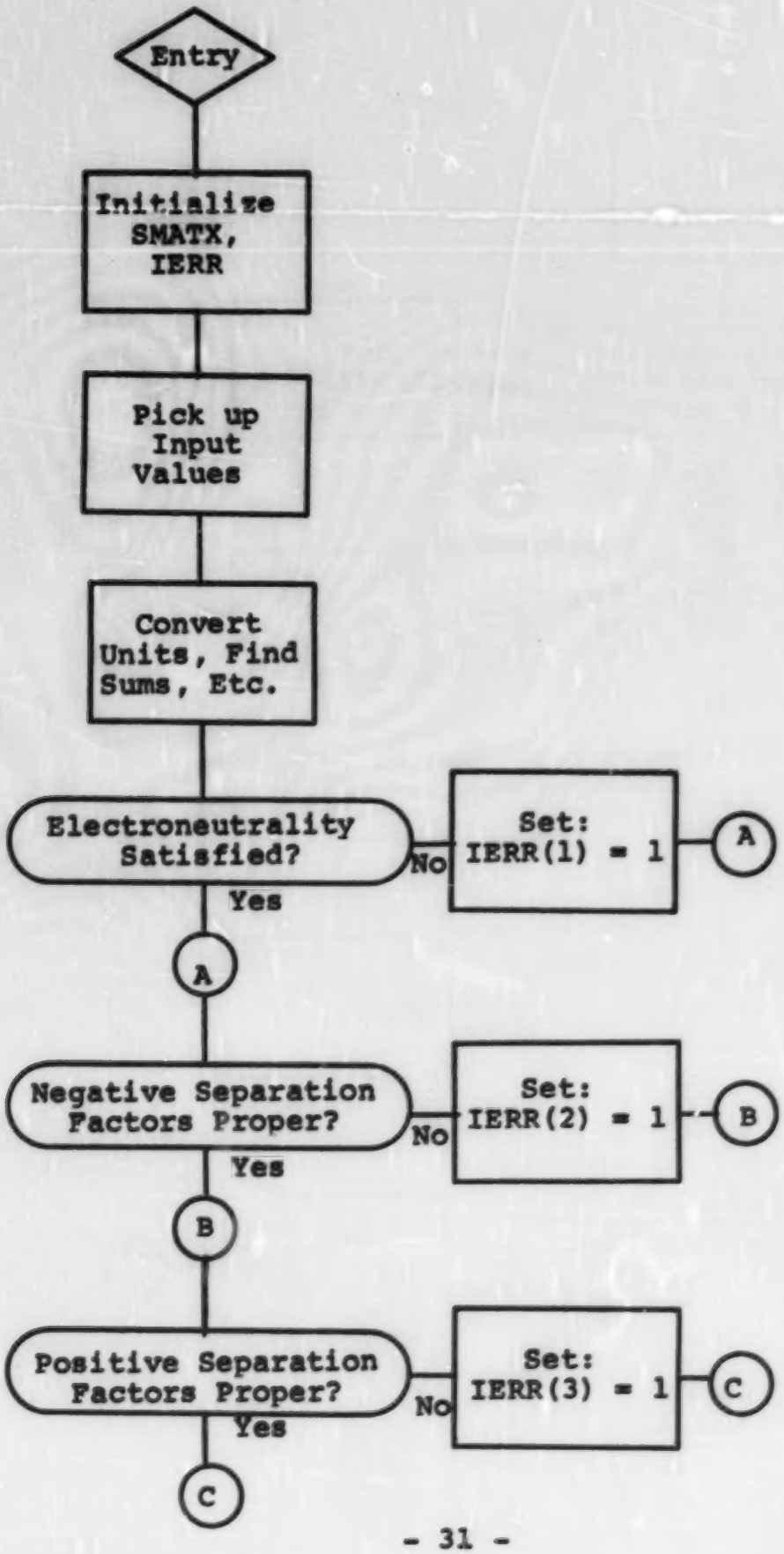
$$ABLDG = 152 + 127.5 \times XNSTK + 20.36 \times Q_3 + 2 \times (Q_3 \times 10^6)^{.33} + (Q_3 \times 10^6)^{.4} \quad (34)$$

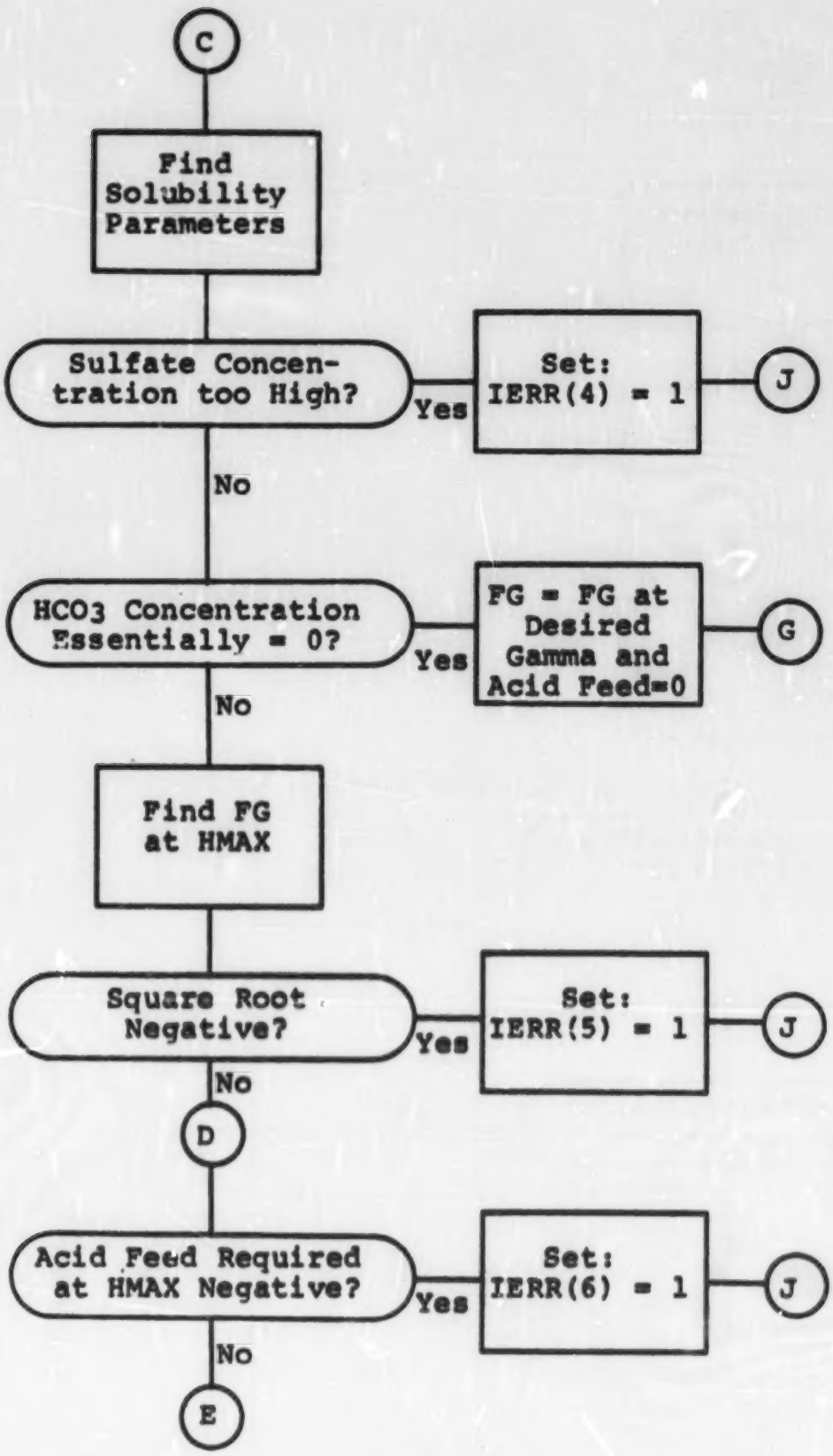
Flow Sheet and Sample Outputs

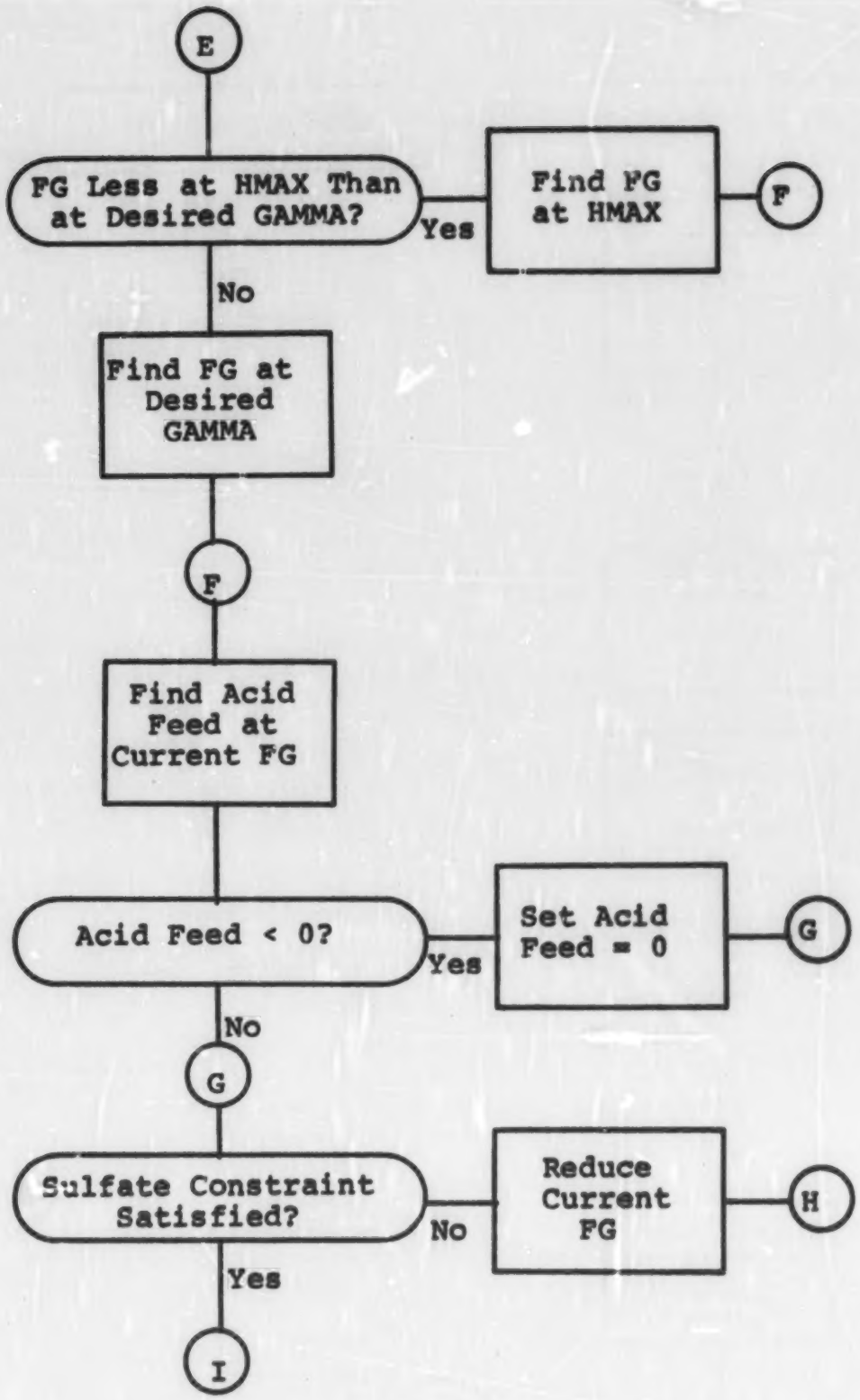
A flow sheet for the computer program ELECT is presented in the following figures, 4 through 6.

Sample outputs from the stand-alone version of the program are given in Tables 1, 2, and 3, for typical secondary effluent compositions and plant capacities of 1, 10 and 100 MGD, respectively.

FLOW DIAGRAM: SUBROUTINE ELECT




C
Find Solubility Parameters
Sulfate Concentration too High?
Yes
Set: IERR(4) = 1
J
No
HCO3 Concentration Essentially = 0?
Yes
FG = FG at Desired Gamma and Acid Feed=0
G
No
Find FG at HMAX
Square Root Negative?
Yes
Set: IERR(5) = 1
J
No
D
Acid Feed Required at HMAX Negative?
Yes
Set: IERR(6) = 1
J
No
E


E
FG Less at HMAX Than at Desired GAMMA?
Yes
Find FG at HMAX
F
No
Find FG at Desired GAMMA
F
Find Acid Feed at Current FG
Acid Feed < 0?
Yes
Set Acid Feed = 0
G
No
G
Sulfate Constraint Satisfied?
No
Reduce Current FG
H
Yes
I

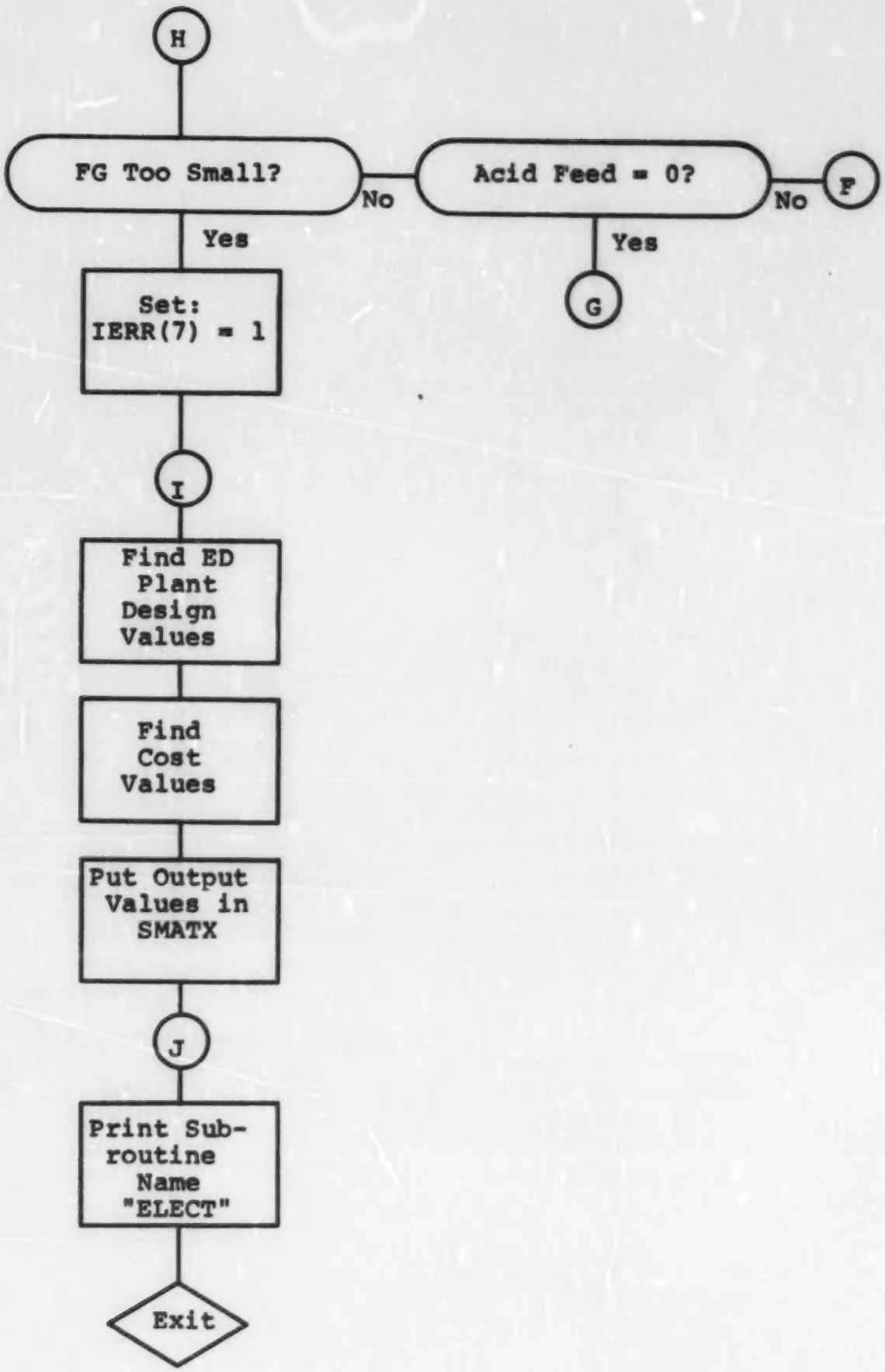

H
FG Too Small?
No
Acid Feed = 0?
No
F
Yes
Yes
G
Set:
IERR(7) = 1
I
Find ED
Plant
Design
Values
Find
Cost
Values
Put Output
Values in
SMATX
J
Print Sub-
routine
Name
"ELECT"
Exit

TABLE 1

Computer Output, 1 MGD Waste Treatment Plant

CONCENTRATION IN	CONCENTRATION OUT	SEPARATION FACTOR	
130.	86.	.79	SODIUM
15.	8.	1.14	POTASSIUM
60.	28.	1.25	CALCIUM
25.	15.	.98	MAGNESIUM
20.	10.	1.15	AMMONIUM
165.	77.	1.25	CHLORIDE
300.	201.	.77	BICARBONATE
100.	53.	1.11	SULFATE
10.	5.	1.22	NITRATE
25.	17.	.72	PHOSPHATE
850.	500.		

.100	SPACER THICKNESS,CM
.100	RATIO OF THICKNESS TO MESH SPACING
70.000	T=WATER TEMPERATURE, DEG F.
40.000	RCM=CATION MEMBRANE RESISTIVITY,OHM-SQ.CM.
40.000	RAM=ANION MEMBRANE RESISTIVITY,OHM-SQ.CM.
.900	E=CURRENT EFFICIENCY
.707	COSINE OF MESH ANGLE,THETA
.083	GAMMA=DESIRED RATIO Q7/Q3
2.000	GMAX=MAXIMUM RATIO Q7/Q3
.001	MAX HYDROGEN ION CONCENTRATION,WASTE STREAM
62.000	LIMITING CURRENT DENSITY PARAMETER,CURK
.010	COST OF ELECTRICITY,$/KWHR

ED POWER-KW	29.9472
STACK HEAD LOSS-FT.H2O	40.3505
TOTAL TRANSFER AREA-SQ.FT.	3602.5841
NUMBER OF STACKS	4
NUMBER OF RECTIFIERS	1
BUILDING AREA-SQ.FT.	1110.0871
FLOW PATH WIDTH-IN.	6.0005
STACK COSTS-$	127830.3481
DC EQPT COSTS-$	12031.3024
AUX EQPT COSTS-$	24756.3443
TOTAL CAPITAL-$	164619.9948
POWER COST-CENTS/KGAL	1.0823
MEMBRANE REPLACEMENT-CENTS/KGAL	2.0822
OTHER OPERATING COST-CENTS/KGAL	3.9093
TOTAL OPERATING COST-CENTS/KGAL	7.0738
INPUT STREAM-MGD	1.0000
PRODUCT STREAM-MGD	.9231
WASTE STREAM-MGD	.0769
ACID FEED-GAL/KGAL WASTE	.3778

EXIT
0"

TABLE 2

Computer Output, 10 MGD Waste Treatment Plant

CONCENTRATION IN	CONCENTRATION OUT	SEPARATION FACTOR	
130.	86.	.79	SODIUM
15.	8.	1.14	POTASSIUM
60.	28.	1.25	CALCIUM
25.	15.	.98	MAGNESIUM
20.	10.	1.15	AMMONIUM
165.	77.	1.25	CHLORIDE
300.	201.	.77	BICARBONATE
100.	53.	1.11	SULFATE
10.	5.	1.22	NITRATE
25.	17.	.72	PHOSPHATE
850.	500.		

.100	SPACER THICKNESS,CM
.100	RATIO OF THICKNESS TO MESH SPACING
70.000	T=WATER TEMPERATURE, DEG F.
40.000	RCM=CATION MEMBRANE RESISTIVITY,OHM-SQ.CM.
40.000	RAM=ANION MEMBRANE RESISTIVITY,OHM-SQ.CM.
.900	E=CURRENT EFFICIENCY
.707	COSINE OF MESH ANGLE,THETA
.083	GAMMA=DESIRED RATIO Q7/Q3
2.000	GMAX=MAXIMUM RATIO Q7/Q3
.001	MAX HYDROGEN ION CONCENTRATION,WASTE STREAM
82.000	LIMITING CURRENT DENSITY PARAMETER,CURK
.010	COST OF ELECTRICITY,$/KWHR

ED POWER-KW	299.4718
STACK HEAD LOSS-FT.H2O	40.3505
TOTAL TRANSFER AREA-SQ.FT.	36025.8406
NUMBER OF STACKS	40
NUMBER OF RECTIFIERS	10
BUILDING AREA-SQ.FT.	6448.7172
FLOW PATH WIDTH-IN.	6.0005
STACK COSTS-$	1113064.7588
DC EQPT COSTS-$	120313.0242
AUX EQPT COSTS-$	89335.6271
TOTAL CAPITAL-$	1322713.4101
POWER COST-CENTS/KGAL	1.0823
MEMBRANE REPLACEMENT-CENTS/KGAL	2.0822
OTHER OPERATING COST-CENTS/KGAL	2.4300
TOTAL OPERATING COST-CENTS/KGAL	5.5945
INPUT STREAM-MGD	10.0000
PRODUCT STREAM-MGD	9.2308
WASTE STREAM-MGD	.7692
ACID FEED-GAL/KGAL WASTE	.3778

TABLE 3

Computer Output, 100 MGD Waste Treatment Plant

CONCENTRATION IN	CONCENTRATION OUT	SEPARATION FACTOR	
130.	86.	.79	SODIUM
15.	8.	1.14	POTASSIUM
60.	28.	1.25	CALCIUM
25.	15.	.98	MAGNESIUM
20.	10.	1.15	AMMONIUM
165.	77.	1.25	CHLORIDE
300.	201.	.77	BICARBONATE
100.	53.	1.11	SULFATE
10.	5.	1.22	NITRATE
25.	17.	.72	PHOSPHATE
850.	500.		

.100	SPACER THICKNESS,CM
.100	RATIO OF THICKNESS TO MESH SPACING
70.000	T=WATER TEMPERATURE, DEG F.
40.000	RCM=CATION MEMBRANE RESISTIVITY,OHM-SQ.CM.
40.000	RAM=ANION MEMBRANE RESISTIVITY,OHM-SQ.CM.
.900	E=CURRENT EFFICIENCY
.707	COSINE OF MESH ANGLE,THETA
.063	GAMMA=DESIRED RATIO Q7/Q3
2.000	GMAX=MAXIMUM RATIO Q7/Q3
.001	MAX HYDROGEN ION CONCENTRATION,WASTE STREAM
82.000	LIMITING CURRENT DENSITY PARAMETER,CURK
.010	COST OF ELECTRICITY,$/KWHR

ED POWER-KW	2994.7179
STACK HEAD LOSS-FT.H2O	40.3505
TOTAL TRANSFER AREA-SQ.FT.	360258.4065
NUMBER OF STACKS	393
NUMBER OF RECTIFIERS	98
BUILDING AREA-SQ.FT.	54524.1120
FLOW PATH WIDTH-IN.	6.1074
STACK COSTS-$	10804862.9849
DC EQPT COSTS-$	1190010.4918
AUX EQPT COSTS-$	649901.3938
TOTAL CAPITAL-$	12644774.8784
POWER COST-CENTS/KGAL	1.0823
MEMBRANE REPLACEMENT-CENTS/KGAL	2.0453
OTHER OPERATING COST-CENTS/KGAL	1.6556
TOTAL OPERATING COST-CENTS/KGAL	4.7837
INPUT STREAM-MGD	100.0000
PRODUCT STREAM-MGD	92.3077
WASTE STREAM-MGD	7.6923
ACID FEED-GAL/KGAL WASTE	.3778

RECOMMENDATIONS AND SUGGESTIONS

It is our recommendation that a program be promptly initiated to establish the effects of varying degrees of pretreatment and operating conditions upon the process design, and for that matter to establish the optimal design of electrodialysis equipment for waste water treatment applications. Such a program should follow the outline suggested in the Conclusions of our final report under FWPCA Contract No. 14-12-91, "Membrane Fouling Mechanisms in the Electrodialysis Process".

Specifically, this program should include but not necessarily be limited to the following:

1. Quantification of the effects of high temperature (50°C) operation on both fouling rates and membrane area reductions;
2. Further examination of the effects of competetive surface area, in the form of entrained microscopic air bubbles, on membrane fouling rates;
3. Determination of the effects of length and frequency of resting periods, both with and without the addition of enzyme active agents, on stack fouling rates;
4. Determination of operating voltages (above the point of polarization) necessary to prevent fouling and the required additional acid feed to control scale problems.

Finally, the results of this program should be used as the basis for electrodialysis design and operating improvements to be incorporated into the mathematical model presented here.

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APPENDIX A

DERIVATION OF ELECTRODIALYSIS DESIGN EQUATIONS

The areal resistivity (ohm-cm^2) of one cell-pair in an electrodialysis stack is obtained from the summation of the resistivities of the two membranes and a dilute and concentrating compartment, i.e.,

$$R_p = R_m + R_d + R_c. \qquad \text{(A-1)}$$

The resistivity contribution of the membrane-solution interface is included in the membrane resistance term in this model. The resistivities of the two solution compartments are expressed in terms of solution concentrations and compartment thicknesses:

$$R_d = \frac{t_d}{\Lambda C_d} \qquad \text{(A-2)}$$

$$R_c = \frac{t_c}{\Lambda C_c} \qquad \text{(A-3)}$$

where:

t = compartment thickness, cm

Λ = equivalent conductance, mho-L/cm-equiv.

C = solution concentration, equiv/L

and d, c, are subscripts referring to diluting and concentrating compartments, respectively.

Solution concentrations, at any point along the flow path (con-current flow) are described as a function of the fractional salt removed at that point:

$$C_d = C_1(1-f) \tag{A-4}$$

$$C_c = C_5 + C_1 f \tag{A-5}$$

As a general practice, the two compartmental thicknesses are maintained equal and the flow rates through the two compartments are the same:

$$t_d = t_c = TKNS \tag{A-6}$$

$$Q_2 = Q_5 \tag{A-7}$$

The concentrating stream concentration then can be described in terms of the total salt reduction obtained through the process (FRACT) and the outlet concentrate stream concentration (C_7):

$$C_c = C_7 - C_1 * FRACT + C_1 f \tag{A-8}$$

The cell pair resistivity then is obtained by substituting equations A-8, A-6, A-4, A-5 and A-2 into A-1:

$$R_p = R_m + \frac{TKNS}{\Lambda\, C_1}\left[\frac{1}{1-f} + \frac{1}{\frac{C_7}{C_1} - FRACT + f}\right] \tag{A-9}$$

(Note: The term CLAM is used in the program for Λ)

At the effluent end of the process, f = FRACT and $C_1(1\text{-FRACT}) = C_3$. The cell-pair resistivity at this point becomes simply:

$$R_{Po} = R_m + \frac{TKNS}{\Lambda}\left[\frac{1}{C_3} + \frac{1}{C_7}\right] \qquad (A\text{-}10)$$

The averaged resistivity through the entire process is obtained from the integration:

$$R_{Pave} = \frac{\int_0^{FRACT} R_P \, df}{\int_0^{FRACT} df} \qquad (A\text{-}11)$$

Performing this integration results in the expression:

$$R_{Pave} = R_m + \frac{TKNS}{FRACT*\Lambda*C_1} \ln\left[\frac{C_7/C_1}{(1\text{-FRACT})\left(\frac{C_7}{C_1}\text{-FRACT}\right)}\right] \qquad (A\text{-}12)$$

Generalized models for predicting the mass (salt) transfer characteristics and pumping energy requirements for electrodialysis systems have been developed by Process Research, Incorporated, under previous contract with the Office of Saline Water, U. S. Department of the Interior. These models are described in OSW R&D Progress Report No. 325.

Limiting mass transfer rates are described through a so-called polarization parameter, $(i/C_d)_{lim}$, which in turn is expressed as a function of fundamental solution and membrane properties and standard hydrodynamic parameters:

$$\left(\frac{i}{C_d}\right)_{lim} = \frac{2F}{k' \nu^{1/3} \ell \sum_j \frac{\bar{z}_j (t_m - t_s)_j}{(D_j \nu)^{2/3}}} \left(\frac{V_o \ell}{\varepsilon \nu \cos\theta}\right)^{0.6} \qquad \text{(A-13)}$$

where:

i = current density, ma/cm^2

C_d = dilute stream solution concentration, eq/L

F = Faraday's constant, 96,500 coulombs/equivalent

k' = empirical constant

ν = kinematic viscosity, cm^2/sec

ℓ = distance (cm) between supporting strands of membrane support material

t_d = flow path thickness, cm

$\bar{z}_j$ = electrochemical valence of ionic species j

t_{m_j} = transference number of species j in the membrane

t_{s_j} = transference number of species j in the solution

D_j = Fickian diffusion coefficient of species j, cm^2/sec

ε = void fraction of spacer flow path

θ = angle between superficial and actual flow directions

V_o = superficial flow velocity, cm/sec

n = number of cell pairs

a = flow path width, cm

In this model, the term $\left(\frac{V_o \ell}{\varepsilon \nu \cos\theta}\right)$ is the mass transfer Reynolds Number for the electrodialysis process. The membrane and solution properties and the various constant coefficients can be lumped together into one term:

$$CURKV = \frac{2F}{k' \sum_j \frac{\bar{z}_j (t_m - t_s)}{(D_j \nu)^{2/3}} j} \qquad \text{(A-14)}$$

For present commercially available membranes and typical waste water compositions, CURKV is about 1.3.

The polarization parameter then is described in terms of hydrodynamic properties only:

$$\left(\frac{i}{C_d}\right)_{lim} = \frac{1.3}{\nu^{.33}\ell} \left(\frac{V_o \ell}{\varepsilon \nu \cos\theta}\right)^{0.6} \qquad \text{(A-15)}$$

(In the program, the term XICD is used for $(i/C_d)_{lim}$. Also, since F_T/nat_d is used for V_o, CURKV is modified to: CURK = $(10^3)^{0.6}$CURKV = 82).

Pumping energy requirements are obtained from the head loss gradient through the electrodialysis process:

$$\frac{h_L}{L} = \frac{\nu^2}{(\frac{2\varepsilon}{\Omega})^{2.75} \cos\theta} \left[.023\left(\frac{2V_o}{\Omega\nu\cos\theta}\right) + 6.98\times10^{-5}\left(\frac{2V_o}{\Omega\nu\cos\theta}\right)^2\right] \qquad \text{(A-16)}$$

where:

$\frac{h_L}{L}$ = pressure drop across electrodialysis spacer, cm H_2O

Ω = wetted surface area per unit of flow path volume, cm^2/cm^3.

In this model, the terms $\left(\frac{2V_o}{\Omega\nu\cos\theta}\right)$ and $\left(\frac{2\varepsilon}{\Omega}\right)$ are the hydraulic Reynolds Number and hydraulic diameter, respectively. In the program, the term PGRAD is used for $\frac{h_L}{L}$.

APPENDIX B

PROGRAM DESCRIPTION

The computer program is for modeling the electrodialysis process as a unit process in the simulation of advanced waste treatment plants. The program is not intended to design a completely self-contained electrodialysis plant.

There are two versions of the program. One is a subroutine for use with the "Executive Digital Computer Program for Preliminary Design of Wastewater Treatment Systems". The second version is an independent program which is completely self-contained. The two versions are essentially equivalent except for the handling of input and output.

The subroutine version gets input values from the stream matrix SMATX, the decision matrix, DMATX, and from other variables in COMMON. Output values are placed in the stream matrix and in variables in COMMON.

The self-contained version accepts input values from an input file, which could be a punched card deck, and puts output values in an output file, which could be a line printer or other device as appropriate.

Listings of both versions are given below.

Program Organization

The program is composed of six parts. Each part of the program is headed by comment cards.

Part 1 picks up input parameters from the stream matrix, SMATX, and from the decision matrix, DMATX.

Part 2 performs unit conversions such as from ppm to moles/liter, finds summations of concentrations, and finds concentrations of each species in the product water stream. Input stream validity checks, described in detail in the section on error conditions, are also made.

Part 3 finds allowable waste stream concentration and required waste stream acid feed based on bicarbonate and sulfate solubility limitations. The resulting product stream volume is also found.

Part 4 computes the electrodialysis system design parameters required.

Part 5 computes the capital cost values and operating cost values.

Part 6 puts output stream values in stream matrix.

NOTATIONS

Fortran Name	Description
ABLDG	Building area required, sq ft
ACA	Separation factor, calcium
ACL	Separation factor, chloride
AHCO3	Separation factor, bicarbonate
AK	Separation factor, potassium
AMG	Separation factor, magnesium
ANA	Separation factor, sodium
ANH4	Separation factor, ammonium
ANO3	Separation factor, nitrate
APO4	Separation factor, phosphate
ASO4	Separation factor, sulfate
CAC	Acid feed required, equivalent acid/l waste
CADI	Calcium concentration, mole/l
CAUX or CCOST(3,N)	Auxillary capital costs, $
CDC or CCOST(2,N)	D.C. related capital costs, $
CDI	Input stream concentration, equivalent/l
CLAM or Λ	Specific solution conductance, mhos/cm per equivalent/l
CLDI	Chloride concentration, mole/l
CPWR or COSTO(1,3)	Power cost, $/yr
CREP or COSTO(2,N)	Membrane replacement, $/yr
CO3K1	Ratio XCACO3/(XK1*XK2) where XCACO3 = calcium carbonate solubility product XK2 = second bicarbonate protolysis constant
COTHE	Cosine of mesh angle, theta

NOTATIONS

Fortran Name	Description
COT or COSTO(3,N)	Other operating cost, $/yr
CSTK or CCOST(1,N)	Stack related capital costs, $
CURK	Limiting current density parameter
EDPWR	D.C. power required for electrodialysis
E	Current efficiency
FG	FRACT/GAMMA (Variable)
FGMAX	FRACT/desired GAMMA
FGMIN	FRACT/maximum GAMMA
FRACT	Fraction demineralized
GAMMA	Volume ratio of waste stream to product stream
GMAX	Maximum allowable waste/product stream volume ratio
HCO	Hydrogen ion concentration, waste stream, mole/l
HCO3D	Bicarbonate concentration, mole/l
HMAX	Max allowable hydrogen ion concentration in waste stream, mole/l
IERR	Error indicator array; values defined below

The following table defines the meaning of the various error indications. If the element listed in the table below is set = 1, the error condition corresponding to that item exists

ELEMENT	Meaning if IERR(I)=1
IERR(1)	The difference betwen SMP and SMN exceeds 5% of SMP. Electroneutrality is violated.

NOTATIONS

Fortran Name	Description
IERR(2)	The difference between SMN and SMCAN is not within 5% of SMN. Negative separation factors are improper.
IERR(3)	The difference between SMP and SMCAP is not within 5% of SMP. Positive separation factors are improper.
IERR(4)	Calcium sulfate solubility product is exceeded by input stream concentrations.
IERR(5)	Negative square root was attempted in quadratic solution for acid feed rate at limiting waste hydrogen ion concentration.
IERR(6)	Minimum brine stream pH (HMAX) is violated even at zero acid feed.
IERR(7)	Calcium sulfate solubility is exceeded even at the minimum brine stream concentration (GMAX).
NSTK	Number of stacks
NRECT	Number of rectifiers
PCA	Input stream concentration of calcium, ppm
PCL	Input stream concentration of chloride, ppm
PHCO3	Input stream concentration of bicarbonate, ppm
PK	Input stream concentration of potassium, ppm
PMG	Input stream concentration of magnesium, ppm
PNA	Input stream concentration of sodium, ppm
PNH4	Input stream concentration of ammonium, ppm
PNO3	Input stream concentration of nitrate, ppm
PO4DI	Phosphate concentration, mole/l
POCA	Product stream concentration of calcium, ppm

NOTATIONS

Fortran Name	Description
POCL	Product stream concentration of chloride, ppm
POHCO	Product stream concentration of bicarbonate, ppm
POK	Product stream concentration of potassium, ppm
POMG	Product stream concentration of magnesium, ppm
PONA	Product stream concentration of sodium, ppm
PONH4	Product stream concentration of ammonia, ppm
PONO3	Product stream concentration of nitrate, ppm
POPO4	Product stream concentration of phosphate, ppm
POSO4	Product stream concentration of sulfate, ppm
PPMO4	Total dissolved inorganic solids, product stream, ppm
PPO4	Input stream concentration of phosphate, ppm
PSO4	Input stream concentration of sulfate, ppm
Q1	Input stream flow, mgd
Q3	Product water flow, mgd
Q7	Waste stream flow, mgd
Q9	Acid feed rate, gal. acid/k gal. waste
RAM	Anion membrane resistivity ohm-sq cm
RCM	Cation membrane resistivity ohm-sq cm
SMCAN	Sum of the products of the equivalents of each negative species with its separation factor

NOTATIONS

Fortran Name	Description
SMCAP	Sum of the products of the equivalents of each positive species with its separation factor
SMN	Sum of the equivalents of each negative species
SMP	Sum of the equivalents of each positive species
SO4DI	Sulfate concentration, mole/l
STKHD	Stack headloss, ft - H_2O (includes manifold loss)
T	Input stream temperature, ^oF
TDBL	Ratio of spacer thickness to mesh spacing
TKNS	Membrane spacing thickness, cm
TTA	Total membrane transfer area required, sq ft
VISC or ν	Kinematic viscosity of water, sq cm/sec
WIDTH	Flow path width, in.
WMCA	Molecular weight, calcium
WMCL	Molecular weight, chloride
WMHCO	Molecular weight, bicarbonate
WMK	Molecular weight, potassium
WMMG	Molecular weight, magnesium
WMNA	Molecular weight, sodium
WMNH4	Molecular weight, ammonium ion
WMNO3	Molecular weight, nitrate
WMPO4	Molecular weight, phosphate
WMSO4	Molecular weight, sulfate
XCASO	Calcium sulfate solubility product

NOTATIONS

Fortran Name	Description
XFTNA	Flow parameter, 1/sec/cm
XK1	First bicarbonate protolysis constant
XKDI	Potassium concentration, mole/l
XKW	Dissociation constant for water
XMGDI	Magnesium concentration, mole/l
XNH4D	Ammonium concentration, mole/l
XNADI	Sodium concentration, mole/l
XNO3D	Nitrate concentration, mole/l
$\wedge$	See CLAM
$\vee$	See VISC

Listings

Following are listings of the source code for both versions of the program and a listing of the data file used for the sample cases.

```
      SUBROUTINE ELECT
      COMMON/EDERR/ XCASO,SMP,SMN,SMCAP,SMCAN,IERR(7)
      COMMON/EDJP/ ABLDG,NSTK,NRECT,EDPWR,STKHD,TTA,WIDTH,99
      DO 5 I=1,7
5     IERR(I)=0
      DO 6 I=1,NROWS
      SMATX(I,OS1)=SMATX(I,IS1)
6     SMATX(I,OS2)=SMATX(I,IS1)
      SMATX(2,OS1)=0.
C
C     PART 1-  PICK UP INPUT PARAMETERS
C
      Q1=SMATX(2,IS1)*DMATX(16,N)
      CKWH=DMATX(1,20)
      PPMOU=DMATX(  ,N)
      TKNS=DMATX(  ,N)
      TDEL=DMATX(  ,N)
      T=DMATX(  ,N)
      RCM=DMATX(  ,N)
      RAM=DMATX(  ,N)
      E=DMATX(  ,N)
      CURK=DMATX(  ,N)
      GAMMA=DMATX(  ,N)
      GMAX=DMATX(  ,N)
      HMAX=DMATX(  ,N)
      COTHE=DMATX(  ,N)
     ANA=DMATX(  ,N)
     AK=DMATX(  ,N)
     ACA=DMATX(  ,N)
     AMG=DMATX(  ,N)
     ANH4=DMATX(  ,N)
     ACL=DMATX(  ,N)
     AHCO3=DMATX(  ,N)
     ASO4=DMATX(  ,N)
     ANO3=DMATX(  ,N)
     APO4=DMATX(  ,N)
      PNA=SMATX(  ,IS1)
      PK=SMATX(  ,IS1)
      PCA=SMATX(  ,IS1)
      PMG=SMATX(  ,IS1)
      PNH4=SMATX(  ,IS1)
      PCL=SMATX(  ,IS1)
      PHCO3=SMATX(  ,IS1)
      PSO4=SMATX(  ,IS1)
      PNO3=SMATX(  ,IS1)
      PPO4=SMATX(  ,IS1)
C
C     PART 2- PERFORM UNIT CONVERSIONS, PPM TO MOL/LTR, ETC.
C             SUM CONCENTRATION VALUES,ETC.
C
      WMNA=22.9898E3
       WMK=39.102E3
      WMCA=40.08E3
      WMMG=24.312E3
```

```
      WMCL=35.453E3
      WMNH4=18.03858E3
       WMHCO =61.0094E3
      WMSO4=96.0616E3
      WMNO3=62.0049E3
      WMPO4=84.949E3
       XNADI=PNA/WMNA
      XKDI=PK/WMK
      CADI=PCA/WMCA
      XMGDI=PMG/WMMG
      CLDI=PCL/WMCL
      XNH4D=PNH4/WMNH4
       HCO3D =PHCO3/WMHCO
       SO4DI=PSO4/WMSO4
       XNO3D =PNO3/WMNO3
      PO4DI=PPO4/WMPO4
       SMP=XNADI+XKDI+2.*CADI+2.*XMGDI   + XNH4D
       SMN=CLDI+HCO3D +2.*SO4DI+XNO3D   + PO4DI * 1.5
       PPMT=PNA+PK+PCA+PMG+PCL+PHCO3+PSO4+PNO3 + PPO4  +PNH4
       SUMCI=SMP-SMN+HCO3D
       SMCAP=ANA*XNADI+AK*XKDI+ACA*CADI*2.+AMG*XMGDI*2.+ANH4*XNH4D
       SMCAN=ACL*CLDI+ASO4*SO4DI*2.+
     1      ANO3*XNO3D+HCO3D*AHCO3+APO4*PO4DI*1.5
      CDI =.5*(SMP+SMN)
      CIAI = ANA*PNA + AK*PK + ACA*PCA + AMG*PMG +ANH4*PNH4 +
     1       ACL*PCL + AHCO3*PHCO3 + ASO4*PSO4 + ANO3*PNO3+APO4*PPO4
      SMCIA =SMCAP-SMCAN+HCO3D *AHCO3
      FRACT = (PPMT - PPMOU )/CIAI
      FGMAX=FRACT/GAMMA
      PONA=PNA*(1.-FRACT*ANA)
      POK=PK*(1.-FRACT*AK)
      POMG=PMG*(1.-FRACT*AMG)
      POCL=PCL*(1.-FRACT*ACL)
      PONH4=PNH4*(1.-FRACT*ANH4)
      POHCO =PHCO3*(1.-FRACT*AHCO3)
      POSO4=PSO4*(1.-FRACT*ASO4)
      PONO3=PNO3*(1.-FRACT*ANO3)
      POCA=PCA*(1.-FRACT*ACA)
      POPO4=PPO4*(1.-FRACT*APO4)
      TPOUT=PONA+POK+POCA+POMG+PONH4+POCL+POHCO+POSO4+PONO3+POPO4
C
C     ERROR CHECK INPUT VALUES
C
      IF(ABS(SMP-SMN)-.05*SMP)832,832,830
830   CONTINUE
      IERR(1)=1
832   CONTINUE
      IF(ABS(SMN-SMCAN)-.05*SMN)835,835,833
833   IERR(2)=1
835   IF(ABS(SMP-SMCAP)-.05*SMP)838,838,836
836   IERR(3)=1
838   CONTINUE
C
C     PART 3- FIND ALLOWABLE WASTE STREAM CONCENTRATION AND
```

```
C           WASTE STREAM ACID FEED BASED ON SULFATE AND
C           BICARBONATE CONCENTRATION.
C
      IF(T-85.)7110,7110,7120
7110    XKW   = .13E-14*(2.3)**((T-32.)/18.)
      GO TO 7150
7120    IF(113.-T) 7130,7130,7140
7130    XKW   = 4.0E-14*(4.0)**((T-113.)/45.)
      GO TO 7150
7140    XKW   = 1.47E-14*(2.72)**((T-86.)/27.)
7150  CONTINUE
      IF(T-70.) 7210,7210,7220
7210    XCASO  = ((1.9+0.2*(T-40.)/30.)/136.)**2
      GO TO 7270
7220    IF(T-103.)7230,7230,7240
7230    XCASO  = 2.4E-4
      GO TO 7270
7240    IF(T-130.) 7250,7250,7260
7250    XCASO  = (2.15*(0.7953488)**((T-100.)/30.)/136.)**2
      GO TO 7270
7260    XCASO  = (1.71*(0.7427)**((T-130.)/30.)/136.)**2
7270   CONTINUE
      CO3K1 =10.** ((12343.5/(T+491.7))-26.75555+.023568*(T+491.7))
      A = 20.9176
      B = -.04803
      C = 3.94298E-5
      HCARB = -.01+A+B*(T+491.7)+C*(T+491.7)**2
      XK1 = 10.**(-HCARB)
C
C     CHECK SULFATE CONSTRAINT TO SEE IF IT MAY BE BINDING
C
      IF(CADI*SO4DI-XCASO )619,617,617
617   IERR(4)=1
      GO TO 1000
619   CONTINUE
      GMP=.95
      IACID=1
      FGMIN=FRACT/GMAX
      IF(CADI*HCO3D-1.E-30)505,505,510
505   FG=FGMAX
      CAC=0.
      IACID=2
      GO TO 650
C
C     CHECK TO SEE IF HMAX LIMITS HCO3 CONCENTRATION
C
510   C1F2=ACA*AHCO3
      C2F2=ACA+AHCO3
20    C3F2=CO3K1 /(CADI*HCO3D )
C
C     SOLVE CASE 1
C     HCO=HMAX, FGAM FROM EQN 2
      S=1.-(C3F2*HMAX*(XK1+HMAX))
      S=C2F2**2-4.*C1F2*S
```

```
      IF (S) 110, 130, 130
110   IERR(5)=1
      GO TO 1000
130   FG=(-C2F2+SQRT(S))/(2.*C1F2)
      CAC=SUMCI+FG*SMCIA -XK1*HCO3D *(1.+
     1    FG*AHCO3)/(XK1+HMAX)+HMAX-XKW/HMAX
C
C     IF CAC IS NEGATIVE=ERROR
C
      IF (CAC) 140,155,155
140   IERR(6)=1
      GO TO 1000
155   IF(FG-FGMAX)520,520,515
515   FG=FGMAX
C
C     FIND H TO SATISFY HCO3 FOR CURRENT FG
C      (THIS IS RE-ENTRY FROM 671.) FIND CAC REQUIRED.
C
520   B=XK1
      C=-(FG*FG*ACA*AHCO3+FG*(ACA+AHCO3)+1.)*CADI*HCO3D /CO3K1
      HCO=(-B+SQRT(B*B-4.*C))/2.
      IF(HCO-1.E-35)640,640,630
C
C     IF HCO IS 'ESSENTIALLY' ZERO THIS CONSTRAINT CAN'T BIND
C
630   CONTINUE
      CAC=SUMCI+FG*SMCIA -XK1*HCO3D *(1.+FG*AHCO3)/(XK1+HCO)
     1     +HCO-XKW/HCO
      IF(CAC)640,640,650
640   CAC=0.
      IACID=2
650   CONTINUE
C
C     NOW HAVE FG,CAC DESIRED FOR HCO3 (AND HMAX).
C     MAY HAVE TO ADJUST DOWN TO SATISFY SO4.
C       (THIS IS FG RE-ENTRY FOR CAC=0.)
C
      XLM=FG*FG*ACA*ASO4*CADI*SO4DI+FG*((ACA+ASO4)*CADI*SO4DI
     1     +CADI*ACA*CAC)+CADI*SO4DI+CADI*CAC-XCASO
      IF(XLM)470,470,660
C
C     IF XLM IS NOT>0 SO4 CONSTRAINT IS SATISFIED.
C
C    TRY REDUCING FG BUT NOT BELOW FGMIN
C
660   IF(FG-FGMIN)665,665,670
665   IERR(7)=1
      GO TO 470
670   FG = FG*GMP
671   GO TO (520,650),IACID
470   CONTINUE
      CMAX = CDI * (1.+FG)
      Q7=Q1/(FG/FRACT+1.)
      Q3=Q1-Q7
```

```
      Q9=Q7*CAC/34.7
C     THE CONSTANT ABOVE, 34.7, IS BASED ON 93%H2S04
C
C
C     PART 4- COMPUTE ELECTRODIALYSIS SYSTEM DESIGN VALUES
C
      FT = Q3 * 43.8079
C      XFTNA=FLOW PARAMETER- FT/NA, LTR/SEC/CM
      XFTNA=2.412E-3
      CLAM = 0.1*EXP(.011*(T-68.))
      VISC = .01*EXP(-.011*(T-68.))
      RM = (RAM+RCM)*EXP(-.011*(T-68.))
      SOL = CDI/CMAX
      CURLI =CURK*TDEL**.4/((VISC**.93)*((1.-.393*
     1TDEL)*COTHE)**.6)
      RN=XFTNA*1000/((1.+TDEL)*VISC*COTHE)
      HDIAM=TKNS*(1-3.14159265*TDEL/8)/(1+TDEL)
      PGRAD=VISC**2*(.023*RN+6.98E-5*RN**2)/(HDIAM**2.75*COTHE)
      XICD=CURLI /TKNS*XFTNA**.6
       RPO=RM+TKNS/(CLAM*CDI)*(1./(1.-FRACT)+SOL)
       XKPP=9.65E+07*(FRACT*RM+TKNS/(CLAM*CDI)*
     1 ALOG (1./((1.-FRACT)*(1.-FRACT*SOL))))/(E*RPO*(1.-FRACT))
       XKP=96.5*CDI**2*FRACT*(1.-FRACT)/E
       XNAP= XKPP/XICD*FT
       EDPWR=XKP*RPO*XICD*FT/1000.
      PMH2O=PGRAD*XNAP/FT*XFTNA/100.
      STKHD=3.281*PMH2O+30.
      TTA = XNAP * 1.0764E-3
      CURDE =96500.*CDI*FRACT*FT/E/TTA
      ELL=TKNS/TDEL*.3937
      XNA=FT/XFTNA
      NSTK=TTA/917.+.9
      XNSTK=NSTK
      NRECT=XNSTK/4.+.5
      IF(NRECT)13,13,14
13    NRECT=1
14    CONTINUE
      WIDTH=XNA*.3937/(XNSTK*275.)
C
C     PART 5- COMPUTE COST VALUES
C
      CCOST(1,N)=27330.*XNSTK+(16800.+38.08*Q3*(STKHD))*Q3**(-.2)
      CCOST(2,N)=1874.25*XNSTK+151.41*EDPWR
      CCOST(3,N)=15993.6+149.79E6*Q9+245.9*Q9**.715
     1      +1102.5*XNSTK*(XNSTK/4.)**(-.17)
      COSTO(1,N)=(2780.5*STKHD*Q3+9733.3333*EDPWR)*CKWH
      COSTO(2,N)=1900.*XNSTK
      COSTO(3,N)=83.44E6*Q9+11268.*Q1**.725+.0035*(CCOST(1,N)+
     1       CCOST(2,N)+CCOST(3,N))
      ASLDG=152.+127.5*XNSTK+20.36*Q3+2.*(Q3*1.E6)**.33+(Q3*1.E6)**.4
      GAMMA=FRACT/FG
C
C     PART 6- PUT OUTPUT STREAM VALUES IN OUTPUT MATRIX,ETC.
C
```

```
      SMATX(   ,OS1)=PONA
      SMATX(   ,OS1)=POK
      SMATX(   ,OS1)=POCA
      SMATX(   ,OS1)=POMG
      SMATX(   ,OS1)=PONH4
      SMATX(   ,OS1)=POCL
      SMATX(   ,OS1)=POHCO3
      SMATX(   ,OS1)=POSO4
      SMATX(   ,OS1)=PONO3
      SMATX(   ,OS1)=POPO4
      SMATX(2,OS1)=Q3
      SMATX(   ,OS2)=(PNA-PONA)/GAMMA
      SMATX(   ,OS2)=(PK-POK)/GAMMA
      SMATX(   ,OS2)=(PCA-POCA)/GAMMA
      SMATX(   ,OS2)=(PMG-POMG)/GAMMA
      SMATX(   ,OS2)=(PNH4-PONH4)/GAMMA
      SMATX(   ,OS2)=(PCL-POCL)/GAMMA
      SMATX(   ,OS2)=(PHCO3-POHCO3)/GAMMA
      SMATX(   ,OS2)=(PSO4-POSO4)/GAMMA+CAC*WMSO4/2.
      SMATX(   ,OS2)=(PNO3-PONO3)/GAMMA
      SMATX(   ,OS2)=(PPO4-POPO4)/GAMMA
      SMATX(2,OS2)=Q7+Q9
        Q9=(Q9/Q7)*1000.
1000  CONTINUE
199   FORMAT(5X,5HELECT)
      PRINT 199
      RETURN
      END
```

```
      L=5
      IN=2
3     READ(IN,5)PNA,PK,PCA,PMG,PNH4,PCL,PHCO3,PSO4,PNO3,PPO4
      IF(PNA)4,7,4
4     READ(IN,5)ANA,AK,ACA,AMG,ANH4,ACL,AHCO3,ASO4,ANO3,APO4
8      READ(IN,5)QI,PPMOO,TKNS,TDEL,T,RCM,RAM,E,CKWH,CURR
      IF(QI)6,3,6
6     READ(IN,5)GAMMA,GMAX,HMAX,COTHE,PRNT
5     FORMAT(10F7.1)
      WRITE(L,999)
999   FORMAT(1H1)
      WMNA=22.9898E3
       WMK=39.102E3
      WMCA=40.08E3
      WMMG=24.312E3
      WMCL=35.453E3
      WMNH4=18.03858E3
       WMHCO =61.0094E3
      WMSO4=96.0616E3
      WMNO3=62.0049E3
      WMPO4=84.949E3
       XNADI=PNA/WMNA
      XKDI=PK/WMK
      CADI=PCA/WMCA
      XMGDI=PMG/WMMG
      CLDI=PCL/WMCL
      XNH4D=PNH4/WMNH4
       HCO3D =PHCO3/WMHCO
       SO4DI=PSO4/WMSO4
       XNO3D =PNO3/WMNO3
      PO4DI=PPO4/WMPO4
       SMP=XNADI+XKDI+2.*CADI+2.*XMGDI   + XNH4D
       SMN=CLDI+HCO3D +2.*SO4DI+XNO3D   + PO4DI * 1.5
       PPMT=PNA+PK+PCA+PMG+PCL+PHCO3+PSO4+PNO3 + PPO4  +PNH4
       SUMCI=SMP-SMN+HCO3D
       SMCAP=ANA*XNADI+AK*XKDI+ACA*CADI*2.+AMG*XMGDI*2.+ANH4*XNH4D
       SMCAN=ACL*CLDI+ASO4*SO4DI*2.+
     1      ANO3*XNO3D+HCO3D*AHCO3+APO4*PO4DI*1.5
      CDI =.5*(SMP+SMN)
      CIAI = ANA*PNA + AK*PK + ACA*PCA + AMG*PMG +ANH4*PNH4 +
     1       ACL*PCL + AHCO3*PHCO3 + ASO4*PSO4 + ANO3*PNO3+APO4*PPO4
      SMCIA =SMCAP-SMCAN+HCO3D *AHCO3
      FRACT = (PPMT - PPMOO )/CIAI
      FGMAX=FRACT/GAMMA
      PONA=PNA*(1.-FRACT*ANA)
      POK=PK*(1.-FRACT*AK)
      POMG=PMG*(1.-FRACT*AMG)
      POCL=PCL*(1.-FRACT*ACL)
      PONH4=PNH4*(1.-FRACT*ANH4)
      POHCO =PHCO3*(1.-FRACT*AHCO3)
      POSO4=PSO4*(1.-FRACT*ASO4)
      PONO3=PNO3*(1.-FRACT*ANO3)
      POCA=PCA*(1.-FRACT*ACA)
      POPO4=PPO4*(1.-FRACT*APO4)
```

```
      TPOUT=PONA+POK+POCA+POMG+PONH4+POCL+POHCO+POSO4+PONO3+POPO4
C
C     ERROR CHECK INPUT VALUES
C
      IF(ABS(SMP-SMN)-.05*SMP)832,832,830
830   CONTINUE
      WRITE(L,831)
831   FORMAT(44H ELECTRONEUTRALITY IS NOT WITHIN 5% AS GIVEN)
832   CONTINUE
      IF(ABS(SMN-SMCAN)-.05*SMN)835,835,833
833   WRITE(L,834)SMN,SMCAN
834   FORMAT(34H SEPARATION FACTORS IMPROPER.SMN= E12.4,7H SMCAN=E12.4)
835   IF(ABS(SMP-SMCAP)-.05*SMP)838,838,836
836   WRITE(L,837)SMP,SMCAP
837   FORMAT(34H SEPARATION FACTORS IMPROPER.SMP= E12.4,7H SMCAP=E12.4)
838   CONTINUE
      IF(T-85.)7110,7110,7120
7110    XKW  = .13E-14*(2.3)**((T-32.)/18.)
      GO TO 7150
7120    IF(113.-T) 7130,7130,7140
7130    XKW  = 4.0E-14*(4.0)**((T-113.)/45.)
      GO TO 7150
7140    XKW  = 1.47E-14*(2.72)**((T-86.)/27.)
7150  CONTINUE
      IF(T-70.) 7210,7210,7220
7210    XCASO  = ((1.9+0.2*(T-40.)/30.)/136.)**2
      GO TO 7270
7220    IF(T-103.)7230,7230,7240
7230    XCASO  = 2.4E-4
      GO TO 7270
7240    IF(T-130.) 7250,7250,7260
7250    XCASO  = (2.15*(0.7953488)**((T-100.)/30.)/136.)**2
      GO TO 7270
7260    XCASO  = (1.71*(0.7427)**((T-130.)/30.)/136.)**2
7270   CONTINUE
      CO3K1 =10.** ((12343.5/(T+491.7))-26.75555+.023568*(T+491.7))
      A = 20.9176
      B = -.04803
      C = 3.94298E-5
      HCARB = -.01+A+B*(T+491.7)+C*(T+491.7)**2
      XK1 = 10.**(-HCARB)
C
C     CHECK SULFATE CONSTRAINT TO SEE IF IT MAY BE BINDING
C
      IF(CADI*SO4DI-XCASO )619,617,617
617   WRITE(L,618)
618   FORMAT(56H SOLUBILITY PRODUCT OF CALCIUM SULFATE EXCEEDS LIMIT OF
     1      E12.4)
      GO TO 1000
619   CONTINUE
      GMP=.95
      IACID=1
      FGMIN=FRACT/GMAX
      IF(CADI*HCO3D-1.E-30)505,505,510
```

```
505   FG=FGMAX
      CAC=0.
      IACID=2
      GO TO 650
C
C     CHECK TO SEE IF HMAX LIMITS HCO3 CONCENTRATION
C
510   C1F2=ACA*AHCO3
      C2F2=ACA+AHCO3
20    C3F2=CO3K1 /(CADI*HCO3D )
C
C     SOLVE CASE 1
C     HCO=HMAX, FCAN FROM EQN 2
      S=1.-(C3F2*HMAX*(XK1+HMAX))
      S=C2F2**2-4.*C1F2*S
      IF (S) 110, 130, 130
  110 WRITE(L,199)
      WRITE(L,115)
115   FORMAT (31H NEGATIVE SQUARE ROOT IN CASE 1 )
      GO TO 1000
130   FG=(-C2F2+SQRT(S))/(2.*C1F2)
      CAC=SUMCI+FG*SMCIA -XK1*HCO3D *(1.+
     1    FG*AHCO3)/(XK1+HMAX)+HMAX-XKW/HMAX
C
C     IF CAC IS NEGATIVE=ERROR
C
      IF (CAC) 140,155,155
140   WRITE(L,199)
      WRITE(L,150)
150   FORMAT (31H STATED PROBLEM IS NOT FEASIBLE
     1    41H MINIMUM BRINE STREAM PH IS VIOLATED
     2    24H EVEN AT ZERO ACID FEED          )
      GO TO 1000
155   IF(FG-FGMAX)520,520,515
515   FG=FGMAX
C
C     FIND H TO SATISFY HCO3 FOR CURRENT FG
C      (THIS IS RE-ENTRY FROM 671.) FIND CAC REQUIRED.
C
520   B=XK1
      C=-(FG*FG*ACA*AHCO3+FG*(ACA+AHCO3)+1.)*CADI*HCO3D /CO3K1
      HCO=(-B+SQRT(B*B-4.*C))/2.
      IF(HCO-1.E-35)640,640,630
C
C     IF HCO IS 'ESSENTIALLY' ZERO THIS CONSTRAINT CAN'T BIND
C
630   CONTINUE
      CAC=SUMCI+FG*SMCIA -XK1*HCO3D *(1.+FG*AHCO3)/(XK1+HCO)
     1     +HCO-XKW/HCO
      IF(CAC)640,640,650
640   CAC=0.
      IACID=2
650   CONTINUE
C
```

```
C       NOW HAVE FG,CAC DESIRED FOR HCO3 (AND HMAX).
C       MAY HAVE TO ADJUST DOWN TO SATISFY SO4.
C         (THIS IS FG RE-ENTRY FOR CAC=0.)
C
        XLM=FG*FG*ACA*ASO4*CADI*SO4DI+FG*((ACA+ASO4)*CADI*SO4DI
       1      +CADI*ACA*CAC)+CADI*SO4DI+CADI*CAC-XCASO
        IF(XLM)470,470,660
C
C       IF XLM IS NOT>0 SO4 CONSTRAINT IS SATISFIED.
C
C       TRY REDUCING FG BUT NOT BELOW FGMIN
C
660     IF(FG-FGMIN)665,665,670
665     WRITE(L,666)
666     FORMAT(53H SULFATE NOT SATISFIED AT MINIMUM WASTE CONCENTRATION)
        GO TO 470
670     FG = FG*GMP
671     GO TO (520,650),IACID
470     CONTINUE
        CMAX = CDI * (1.+FG)
        Q1=Q1/(FG/FRACT+1.)
        Q3=Q1-Q7
        Q9=Q7*CAC/34.7
C       THE CONSTANT ABOVE, 34.7, IS BASED ON 93%H2SO4
C
199     FORMAT(42H ERROR IN ELECTRODIALYSIS DESIGN PROBLEM     )
        FT = Q3 * 43.8079
C        XFTNA=FLOW PARAMETER- FT/NA, LTR/SEC/CM
        XFTNA=2.412E-3
        CLAM = 0.1*EXP(.011*(T-68.))
        VISC = .01*EXP(-.011*(T-68.))
        RM = (RAM+RCM)*EXP(-.011*(T-68.))
        SOL = CDI/CMAX
        CURLI =CURK*TDEL**.4/((VISC**.93)*((1.-.393*
       1TDEL)*COTHE)**.6)
        RN=XFTNA*1000/((1.+TDEL)*VISC*COTHE)
        HDIAM=TKNS*(1-3.14159265*TDEL/8)/(1+TDEL)
        PGRAD=VISC**2*(.023*RN+6.98E-5*RN**2)/(HDIAM**2.75*COTHE)
        XICD=CURLI /TKNS*XFTNA**.6
         RPO=RM+TKNS/(CLAM*CDI)*(1./(1.-FRACT)+SOL)
         XKPP=9.65E+07*(FRACT*RM+TKNS/(CLAM*CDI)*
       1 ALOG (1./((1.-FRACT)*(1.-FRACT*SOL))))/(E*RPO*(1.-FRACT))
         XKP=96.5*CDI**2*FRACT*(1.-FRACT)/E
         XNAP= XKPP/XICD*FT
         EDPWR=XKP*RPO*XICD*FT/1000.
        PMH2O=PGRAD*XNAP/FT*XFTNA/100.
        STKHD=3.281*PMH2O+30.
        TTA = XNAP * 1.0764E-3
        CURDE =96500.*CDI*FRACT*FT/E/TTA
        ELL=TKNS/TDEL*.3937
        XNA=FT/XFTNA
        NSTK=TTA/917.+.9
        XNSTK=NSTK
        NRECT=XNSTK/4.+.5
```

```
      IF(NREC)13,13,14
13    NREC=1
14    CONTINUE
      WIDTH=XNA*.3937/(XNSTK*275.)
      CSTK=27330.*XNSTK+(16800.+[illegible].08*Q3*(STKHD))*(Q3**(-.2)
      CDC=1[illegible]7.25*XNSTK+151.41*EDPWR
      CAUX=159[illegible]149.79E6*Q9+245.*Q9**.715
     1      +1102.5*XNSTK*(XNSTK/4.)**(-.17)
      CAP=CSTK+CDC+CAUX
      CPWR=(2780.5*STKHD*Q3+9733.3333*EDPWR)*CKWH
      CREP=1900.*XNSTK
      COT=83.[illegible]*Q9+11268.*Q1**.725+.0035*(CSTK+CDC+CAUX)
C
C     OPERATING COSTS IN CENTS/KGAL ARE BASED ON INPUT FLOW SO THAT
C     COST IS PER UNIT OF WASTE WATER TREATED. TO  FIND COST PER UNIT
C     OF USABLE WATER PRODUCED REPLACE Q1 IN THE FOLLOWING EXPRESSIONS
C       WITH Q2
C
      COT=COT/Q1/3650.
      CPWR=CPWR/Q1/3650.
      CREP=CREP/Q1/3650.
      OP=CPWR+COT+CREP
      ABLDG=152.+127.5*XNSTK+20.36*Q3+2.*(Q3*1.E6)**.33+(Q3*1.E6)**.4
1000  CONTINUE
        Q9=(Q9/Q7)*1000.
      IF(PRNT)30,30,21
21    CONTINUE
950   FORMAT(30H    CONCENTRATION    SEPARATION      )
951   FORMAT(30H      IN       OUT      FACTOR       )
952   FORMAT(F8.0,F9.0,F10.2,7H SODIUM )
953   FORMAT(F8.0,F9.0,F10.2,10H POTASSIUM  )
954   FORMAT(F8.0,F9.0,F10.2,8H CALCIUM  )
955   FORMAT(F8.0,F9.0,F10.2,10H MAGNESIUM )
956   FORMAT(F8.0,F9.0,F10.2,9H AMMONIUM  )
957   FORMAT(F8.0,F9.0,F10.2,9H CHLORIDE  )
958   FORMAT(F8.0,F9.0,F10.2,12H BICARBONATE  )
959   FORMAT(F8.0,F9.0,F10.2,8H SULFATE  )
960   FORMAT(F8.0,F9.0,F10.2,8H NITRATE  )
961   FORMAT(F8.0,F9.0,F10.2,10H PHOSPHATE  )
962   FORMAT(F8.0,F9.0  //)
      WRITE(L,950)
      WRITE(L,951)
      WRITE(L,952)PNA,PONA,ANA
      WRITE(L,953)PK,POK,AK
      WRITE(L,954)PCA,POCA,ACA
      WRITE(L,955)PMG,POMG,AMG
      WRITE(L,956)PNH4,PONH4,ANH4
      WRITE(L,957)PCL,POCL,ACL
      WRITE(L,958)PHCO3,POHCO,AHCO3
      WRITE(L,959)PSO4,POSO4,ASO4
      WRITE(L,960)PNO3,PONO3,ANO3
      WRITE(L,961)PPO4,POPO4,APO4
      WRITE(L,962)PPMT,TPOUT
      WRITE(L,963)TKNS
```

```
      WRITE(L,964)TDEL
      WRITE(L,965)T
      WRITE(L,966)RCM
      WRITE(L,967)RAM
      WRITE(L,968)E
      WRITE(L,969)COTHE
      WRITE(L,970)GAMMA
      WRITE(L,971)GMAX
      WRITE(L,972)HMAX
      WRITE(L,973)CURK
      WRITE(L,974)CKWH
963   FORMAT(F10.3,20H SPACER THICKNESS,CM  )
964   FORMAT(F10.3,35H RATIO OF THICKNESS TO MESH SPACING  )
965   FORMAT(F10.3,28H T=WATER TEMPERATURE, DEG F.   )
966   FORMAT(F10.3,43H RCM=CATION MEMBRANE RESISTIVITY,OHM-SQ.CM. )
967   FORMAT(F10.3,43H RAM=ANION  MEMBRANE RESISTIVITY,OHM-SQ.CM. )
968   FORMAT(F10.3,21H E=CURRENT EFFICIENCY )
969   FORMAT(F10.3,27H COSINE OF MESH ANGLE,THETA )
970   FORMAT(F10.3,27H GAMMA=DESIRED  RATIO 07/03 )
971   FORMAT(F10.3,25H GMAX=MAXIMUM RATIO 07/03 )
972   FORMAT(F10.3,44H MAX HYDROGEN ION CONCENTRATION,WASTE STREAM   )
973   FORMAT(F10.3,40H LIMITING CURRENT DENSITY PARAMETER,CURK )
974   FORMAT(F10.3,31H COST OF ELECTRICITY,$/KWHR      //)
30    CONTINUE
      WRITE(L,901)EDPWR
      WRITE(L,902)STKHD
      WRITE(L,903)TTA
      WRITE(L,904)NSTK
      WRITE(L,905)NRECT
      WRITE(L,920)ABLDG
      WRITE(L,906)WIDTH
      WRITE(L,908)CSTK
      WRITE(L,909)CDC
      WRITE(L,910)CAUX
      WRITE(L,918)CAP
      WRITE(L,911)CPWR
      WRITE(L,912)CREP
      WRITE(L,913)COT
      WRITE(L,919)OP
      WRITE(L,914)01
      WRITE(L,915)03
      WRITE(L,916)07
      WRITE(L,917)09
901   FORMAT(32H ED POWER-KW                          F15.4)
902   FORMAT(32H STACK HEAD LOSS-FT.H2O               F15.4)
903   FORMAT(32H TOTAL TRANSFER AREA-SQ.FT.           F15.4)
904   FORMAT(32H NUMBER OF STACKS                     I10)
905   FORMAT(32H NUMBER OF RECTIFIERS                 I10)
906   FORMAT(32H FLOW PATH WIDTH-IN.                  F15.4)
908   FORMAT(32H STACK COSTS-$                        F15.4)
909   FORMAT(32H DC EQPT COSTS-$                      F15.4)
910   FORMAT(32H AUX EQPT COSTS-$                     F15.4)
911   FORMAT(32H POWER COST-CENTS/KGAL                F15.4)
912   FORMAT(32H MEMBRANE REPLACEMENT-CENTS/KGAL      F15.4)
```

```
 913   FORMAT(32H OTHER OPERATING COST-CENTS/KGAL F15.4)
 914   FORMAT(32H INPUT STREAM-MGD                F15.4)
 915   FORMAT(32H PRODUCT STREAM-MGD              F15.4)
 916   FORMAT(32H WASTE STREAM-MGD                F15.4)
 917   FORMAT(32H ACID FEED-GAL/KGAL WASTE        F15.4)
 918   FORMAT(32H TOTAL CAPITAL-$                 F15.4)
 919   FORMAT(32H TOTAL OPERATING COST-CENTS/KGAL F15.4)
 920   FORMAT(32H BUILDING AREA-SQ.FT.            F15.4)
 1001  GO TO 8
 7     CONTINUE
       CALL EXIT
       END
```

THE FOLLOWING IS THE DATA FILE USED TO PRODUCE THE SAMPLE OUTPUTS:

```
130.    15.     60.     25.     20.     165.    300.    100.    10.     25.
.79     1.14    1.25    .98     1.15    1.25    .77     1.11    1.22    .72
10.     500.    .1      .1      70.     40.     40.     .9      .01     82.
.0833332.       .001    .707    1.
100.    500.    .1      .1      70.     40.     40.     .9      .01     82.
.0833332.       .001    .707    1.
1.      500.    .1      .1      70.     40.     40.     .9      .01     82.
.0833332.       .001    .707    1.
```

VARIABLE NAMES: DECISION MATRIX

THE FOLLOWING VARIABLES MUST BE PROVIDED AS INPUT TO THE ELECTRODIALYSIS SUBROUTINE VIA THE DECISION MATRIX, DMATX. THE NAMES LISTED HERE ARE THE FORTRAN VARIABLE NAMES USED WITHIN THE SUBROUTINE.

TEXT NAME	PROGRAM NAME	NOMINAL VALUE	DESCRIPTION
	PPMOU	500	TOTAL DISSOLVED INORGANIC SOLIDS, PRODUCT STREAM, PPM
TKNS	TKNS	.1	MEMBRANE SPACER THICKNESS, CM.
TDEL	TDEL	.1	RATIO OF SPACER THICKNESS TO MESH SPACING
	T	70.	INPUT STREAM TEMPERATURE, DEG-F.
	RCM	40.	CATION MEMBRANE RESISTIVITY, OHM-SQ.CM.
	RAM	40.	ANION MEMBRANE RESISTIVITY, OHM-SQ.CM.
E	E	.9	CURRENT EFFICIENCY
CURK	CURK	82.	LIMITING CURRENT DENSITY PARAMETER
	GAMMA		DESIRED WASTE/PRODUCT STREAM VOLUME RATIO
	GMAX		MAXIMUM ALLOWABLE WASTE/PRODUCT STREAM VOLUME RATIO
	HMAX	.001	MAX ALLOWABLE HYDROGEN ION CONCENTRATION IN WASTE STREAM
	COTHE	.707	COSINE OF MESH ANGLE, THETA
	ANA	.79	SEPARATION FACTOR, SODIUM
	AK	1.14	SEPARATION FACTOR, POTASSIUM
	ACA	1.25	SEPARATION FACTOR, CALCIUM
	AMG	.98	SEPARATION FACTOR, MAGNESIUM
	ANH4	1.15	SEPARATION FACTOR, AMMONIUM
	ACL	1.25	SEPARATION FACTOR, CHLORIDE
	AHCO3	.77	SEPARATION FACTOR, BICARBONATE
	ASO4	1.11	SEPARATION FACTOR, SULFATE
	ANO3	1.22	SEPARATION FACTOR, NITRATE
	APO4	.72	SEPARATION FACTOR, PHOSPHATE

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